SCALE Manual

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SCALE developers

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RADIATION SHIELDING

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CHAPTER

ONE

MAVRIC: MONACO WITH AUTOMATED VARIANCE REDUCTION USING IMPORTANCE CALCULATIONS

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1.1 Introduction

Monte Carlo particle transport calculations for deep penetration problems can require very long run times in order to achieve an acceptable level of statistical uncertainty in the final answers. Discrete-ordinates codes can be faster but have limitations relative to the discretization of space, energy, and direction. Monte Carlo calculations can be modified (biased) to produce results with the same variance in less time if an approximate answer or some other additional information is already known about the problem. If importances can be assigned to different particles based on how much they will contribute to the final answer, then more time can be spent on important particles, with less time devoted to unimportant particles. One of the best ways to bias a Monte Carlo code for a particular tally is to form an importance map from the adjoint flux based on that tally. Unfortunately, determining the exact adjoint flux could be just as difficult as computing the original problem itself. However, an approximate adjoint can still be very useful in biasing the Monte Carlo solution [Wag97]. Discrete ordinates can be used to quickly compute that approximate adjoint. Together, Monte Carlo and discrete ordinates can be used to find solutions to thick shielding problems in reasonable times.

The MAVRIC (Monaco with Automated Variance Reduction using Importance Calculations) sequence is based on the CADIS (Consistent Adjoint Driven Importance Sampling) and FW-CADIS (Forward-Weighted CADIS) methodologies [WH98] [Wag02] [HW03] [WBP07] MAVRIC automatically performs a three-dimensional, discrete-ordinates calculation using Denovo to compute the adjoint flux as a function of position and energy. This adjoint flux information is then used to construct an importance map (i.e., target weights for weight windows) and a biased source distribution that work together—particles are born with a weight matching the target weight of the cell into which they are born. The fixed-source Monte Carlo radiation transport Monaco [Pep11] then uses the importance map for biasing during particle transport, and it uses the biased source distribution as its source. During transport, the particle weight is compared with the importance map after each particle interaction and whenever a particle crosses into a new importance cell in the map.

For problems that do not require variance reduction to complete in a reasonable time, execution of MAVRIC without the importance map calculation provides an easy way to run Monaco. For problems that do require variance reduction to complete in a reasonable time, MAVRIC removes the burden of setting weight windows from the user and performs it automatically with a minimal amount of additional input. Note that the MAVRIC sequence can be used with the final Monaco calculation as either a multigroup (MG) or a continuous-energy (CE) calculation.

Monaco has a wide variety of tally options: it can calculate fluxes (by group) at a point in space, over any geometrical region, or for a user-defined, three-dimensional, rectangular grid. These tallies can also integrate the fluxes with either standard response functions from the cross section library or user-defined response functions. All of these tallies are available in the MAVRIC sequence.

Although it was originally designed for CADIS, the MAVRIC sequence is also capable of creating importance maps using both forward and adjoint deterministic estimates. The FW-CADIS method [WPM14] can be used for optimizing several tallies at once, a mesh tally over a large region, or a mesh tally over the entire problem. Several other methods for producing importance maps are also available in MAVRIC and are explored in *MAVRIC Appendix C: Advanced Features*.

1.2 CADIS Methodology

MAVRIC is an implementation of CADIS (Consistent Adjoint Driven Importance Sampling) using the Denovo SN and Monaco Monte Carlo functional modules. Source biasing and a mesh-based importance map, overlaying the physical geometry, are the basic methods of variance reduction. To make the best use of an importance map, the map must be made consistent with the source biasing. If the source biasing is inconsistent with the weight windows that will be used during the transport process, then source particles will undergo Russian roulette or splitting immediately, wasting computational time and negating the intent of the biasing.

1.2.1 Overview of CADIS

CADIS is well described in the literature, so only a brief overview is given here. Consider a class source-detector problem described by a unit source with emission probability distribution function $q\left(\overrightarrow{r}, E\right)$ and a detector response function $\sigma_d\left(\overrightarrow{r}, E\right)$. To determine the total detector response, *R*, the forward scalar flux $\phi\left(\overrightarrow{r}, E\right)$ must be known. The response is found by integrating the product of the detector response function and the flux over the detector volume V_d:

$$R = \int_{V_d} \int_E \sigma_d\left(\overrightarrow{r}, E\right) \phi\left(\overrightarrow{r}, E\right) dE\, dV. \tag{1.1}$$

Alternatively, if the adjoint scalar flux, $\phi^+\left(\overrightarrow{r}, E\right)$, is known from the corresponding adjoint problem with adjoint source $q^+\left(\overrightarrow{r}, E\right) = \sigma_d\left(\overrightarrow{r}, E\right)$, then the total detector response could be found by integrating the product of the forward source and the adjoint flux over the source volume, V_s:

$$R = \int_{V_s} \int_E q\left(\overrightarrow{r}, E\right) \phi^+\left(\overrightarrow{r}, E\right) dE\, dV. \tag{1.2}$$

Unfortunately, the exact adjoint flux may be just as difficult to determine as the forward flux, but an approximation of the adjoint flux can still be used to form an importance map and a biased source distribution for use in the forward Monte Carlo calculation.

Wagner [Wag97] showed that if an estimate of the adjoint scalar flux for the corresponding adjoint problem can be found, then an estimate of the response *R* can be made using (1.2). The adjoint source for the adjoint problem is typically separable and corresponds to the detector response and spatial area of the tally to be optimized: $q^+\left(\overrightarrow{r}, E\right) = \sigma_d\left(E\right) g\left(\overrightarrow{r}\right)$, where $\sigma_d\left(E\right)$ is a flux-to-dose conversion factor and $g\left(\overrightarrow{r}\right)$ is 1 in the tally volume and is 0 otherwise. Then, from the adjoint flux $\phi^+\left(\overrightarrow{r}, E\right)$ and response estimate *R*, a biased source distribution, $\widehat{q}\left(\overrightarrow{r}, E\right)$, for source sampling of the form

$$\widehat{q}\left(\overrightarrow{r}, E\right) = \frac{1}{R} q\left(\overrightarrow{r}, E\right) \phi^+\left(\overrightarrow{r}, E\right) \tag{1.3}$$

and weight window target values, $\overline{w}\left(\overrightarrow{r}, E\right)$, for particle transport of the form

$$\overline{w}\left(\overrightarrow{r}, E\right) = \frac{R}{\phi^+\left(\overrightarrow{r}, E\right)} \tag{1.4}$$

can be constructed, which minimizes the variance in the forward Monte Carlo calculation of *R*.

When a particle is sampled from the biased source distribution $\widehat{q}\left(\overrightarrow{r}, E\right)$, to preserve a fair game, its initial weight is set to

$$w_0\left(\overrightarrow{r}, E\right) = \frac{q\left(\overrightarrow{r}, E\right)}{\widehat{q}\left(\overrightarrow{r}, E\right)} = \frac{R}{\phi^+\left(\overrightarrow{r}, E\right)} \tag{1.5}$$

which exactly matches the target weight for that particle's position and energy. This is the "consistent" part of CADIS—source particles are born with a weight matching the weight window of the region/energy into which they are born. The source biasing and the weight windows work together.

CADIS has been applied to many problems—including reactor ex-core detectors, well-logging instruments, cask shielding studies, and independent spent fuel storage facility models—and has demonstrated very significant speed-ups in calculation time compared to analog simulations.

1.2.2 Multiple sources with CADIS

For a typical Monte Carlo calculation with multiple sources—each with a probability distribution function $q_i\left(\overrightarrow{r}, E\right)$ and a strength S_i, giving a total source strength of $S = \sum S_i$—the source is sampled in two steps. First, the specific source *i* is sampled with probability $p\left(i\right) = S_i/S$, and then the particle is sampled from the specific source distribution $q_i\left(\overrightarrow{r}, E\right)$.

The source sampling can be biased at both levels: from which source to sample and how to sample each source. For example, the specific source can be sampled using some arbitrary distribution, $\widehat{p}\left(i\right)$, and then the individual sources can be sampled using distributions $\widehat{q}_i\left(\overrightarrow{r}, E\right)$. Particles would then have a birth weight of

$$w_0 \equiv \left(\frac{p\left(i\right)}{\widehat{p}\left(i\right)}\right)\left(\frac{q_i\left(\overrightarrow{r}, E\right)}{\widehat{q}_i\left(\overrightarrow{r}, E\right)}\right). \tag{1.6}$$

For CADIS, a biased multiple source needs to be developed so that the birth weights of sampled particles still match the target weights of the importance map. For a problem with multiple sources—each with a distribution $q_i\left(\overrightarrow{r}, E\right)$ and a strength S_i—the goal of the Monte Carlo calculation is to compute some response R for a response function $\sigma_d\left(\overrightarrow{r}, E\right)$ at a given detector,

$$R = \int_V \int_E \sigma_d\left(\overrightarrow{r}, E\right) \phi\left(\overrightarrow{r}, E\right) dE\, dV. \tag{1.7}$$

Note that the flux $\phi\left(\overrightarrow{r}, E\right)$ has contributions from each source. The response, R_i, from each specific source (S_i with $q_i\left(\overrightarrow{r}, E\right)$) can be expressed using just the flux from that source, $\phi_i\left(\overrightarrow{r}, E\right)$, as

$$R_i = \int_V \int_E \sigma_d\left(\overrightarrow{r}, E\right)\ \phi_i\left(\overrightarrow{r}, E\right) dE\, dV\,. \tag{1.8}$$

The total response is then found as $R = \sum_i R_i$.

For the adjoint problem, using the adjoint source of $q^+\left(\overrightarrow{r}, E\right) = \sigma_d\left(\overrightarrow{r}, E\right)$, the response R can also be calculated as

$$R = \int_V \int_E \left[\sum_i S_i q_i\left(\overrightarrow{r}, E\right)\right]\ \phi^+\left(\overrightarrow{r}, E\right) dE\, dV, \tag{1.9}$$

with the response contribution from each specific source being

$$R_i = \int_V \int_E S_i q_i\left(\overrightarrow{r}, E\right) \phi^+\left(\overrightarrow{r}, E\right) dE\, dV. \tag{1.10}$$

The target weights $\overline{w}\left(\overrightarrow{r}, E\right)$ of the importance map are found using

$$\overline{w}\left(\overrightarrow{r}, E\right) = \frac{R/S}{\phi^+\left(\overrightarrow{r}, E\right)}. \tag{1.11}$$

Each biased source $\widehat{q}_i\left(\overrightarrow{r},E\right)$ pdf is found using

$$\widehat{q}_i\left(\overrightarrow{r},E\right)=\frac{S_i}{R_i}q_i\left(\overrightarrow{r},E\right)\phi^+\left(\overrightarrow{r},E\right)\ , \tag{1.12}$$

and the biased distribution used to select an individual source is $\widehat{p}\left(i\right)=\ R_i/\sum R_i=R_i/R$.

When using the biased distribution used to select an individual source, $\widehat{p}\left(i\right)$, and the biased source distribution, $\widehat{q}_i\left(\overrightarrow{r},E\right)$, the birth weight of the sampled particle will be

$$\begin{aligned} w_0 &\equiv \left(\frac{p(i)}{\widehat{p}(i)}\right)\left(\frac{q_i\left(\overrightarrow{r},E\right)}{\widehat{q}_i\left(\overrightarrow{r},E\right)}\right) \\ &= \left(\frac{\frac{S_i}{S}}{\frac{R_i}{R}}\right)\left(\frac{q_i\left(\overrightarrow{r},E\right)}{\frac{S_i}{R_i}q_i\left(\overrightarrow{r},E\right)\phi^+\left(\overrightarrow{r},E\right)}\right) \\ &= \frac{R/S}{\phi^+\left(\overrightarrow{r},E\right)}, \end{aligned} \tag{1.13}$$

which matches the target weight, $\overline{w}\left(\overrightarrow{r},E\right)$.

1.2.3 Multiple tallies with CADIS

The CADIS methodology works quite well for classic source/detector problems. The statistical uncertainty of the tally that serves as the adjoint source is greatly reduced since the Monte Carlo transport is optimized to spend more simulation time on those particles that contribute to the tally, at the expense of tracking particles in other parts of phase space. However, more recently, Monte Carlo has been applied to problems in which multiple tallies need to all be found with low statistical uncertainties. The extension of this idea is the mesh tally—where each voxel is a tally for which the user desires low statistical uncertainties. For these problems, the user must accept a total simulation time that is controlled by the tally with the slowest convergence and simulation results where the tallies have a wide range of relative uncertainties.

The obvious way around this problem is to create a separate problem for each tally and use CADIS to optimize each. Each simulation can then be run until the tally reaches the level of acceptable uncertainty. For more than a few tallies, this approach becomes complicated and time-consuming for the user. For large mesh tallies, this approach is not reasonable.

Another approach to treat several tallies, if they are in close proximity to each other, or a mesh tally covering a small portion of the physical problem, is to use the CADIS methodology with the adjoint source near the middle of the tallies to be optimized. Since particles in the forward Monte Carlo simulation are optimized to reach the location of the adjoint source, all the tallies surrounding that adjoint source should converge quickly. This approach requires the difficult question of "how close." If the tallies are too far apart, then certain energies or regions that are needed for one tally may be of low importance for getting particles to the central adjoint source. This may under-predict the flux or dose at the tally sites far from the adjoint source.

MAVRIC has the capability to have multiple adjoint sources with this problem in mind. For several tallies that are far from each other, multiple adjoint sources could be used. In the forward Monte Carlo, particles would be drawn to one of those adjoint sources. The difficulty with this approach is that typically the tally that is closest to the true physical source converges faster than the other tallies——showing that the closest adjoint source seems to attract more particles than the others. Assigning more strength to the adjoint source further from the true physical source helps to address this issue, but finding the correct strengths so that all of the tallies converge to the same relative uncertainty in one simulation is an iterative process for the user.

1.2.4 Forward-weighted CADIS

To converge several tallies to the same relative uncertainty in one simulation, the adjoint source corresponding to each of those tallies must be weighted inversely by the expected tally value. To calculate the dose rate at two points——say one near a reactor and one far from a reactor——in one simulation, then the total adjoint source used to develop the weight windows and biased source must have two parts. The adjoint source far from the reactor must have more strength than the adjoint source near the reactor by a factor equal to the ratio of the expected near dose rate to the expected far dose rate.

This concept can be extended to mesh tallies, as well. Instead of using a uniform adjoint source strength over the entire mesh tally volume, each voxel of the adjoint source should be weighted inversely by the expected forward tally value for that voxel. Areas of low flux or low dose rate would have more adjoint source strength than areas of high flux or high dose rate.

An estimate of the expected tally results can be found by using a quick discrete-ordinates calculation. This leads to an extension of the CADIS method: forward-weighted CADIS (FW-CADIS). First, a forward S_N calculation is performed to estimate the expected tally results. A total adjoint source is constructed so that the adjoint source corresponding to each tally is weighted inversely by those forward tally estimates. Then the standard CADIS approach is used—an importance map (target weight windows) and a biased source are made using the adjoint flux computed from the adjoint S_N calculation.

For example, if the goal is to calculate a detector response function $\sigma_d(E)$ (such as dose rate using flux-to-dose-rate conversion factors) over a volume (defined by $g(\overrightarrow{r})$) corresponding to mesh tally, then instead of simply using $q^+(\overrightarrow{r}, E) = \sigma_d(E)\ g(\overrightarrow{r})$, the adjoint source would be

$$q^+(\overrightarrow{r}, E) = \frac{\sigma_d(E)\,\mathrm{g}(\overrightarrow{r})}{\int \sigma_d(E)\,\phi(\overrightarrow{r}, E)dE}\,, \tag{1.14}$$

where $\phi(\overrightarrow{r}, E)$ is an estimate of the forward flux, and the energy integral is over the voxel at $\overrightarrow{r}$. The adjoint source is nonzero only where the mesh tally is defined ($g(\overrightarrow{r})$), and its strength is inversely proportional to the forward estimate of dose rate.

The relative uncertainty of a tally is controlled by two components: (1) the number of tracks contributing to the tally and (2) the shape of the distribution of scores contributing to that tally. In the Monte Carlo game, the number of simulated particles, $m(\overrightarrow{r}, E)$, can be related to the true physical particle density, $n(\overrightarrow{r}, E)$, by the average Monte Carlo weight of scoring particles, $\overline{w}(\overrightarrow{r}, E)$, by

$$n(\overrightarrow{r}, E) = \overline{w}(\overrightarrow{r}, E)\,\mathrm{m}(\overrightarrow{r}, E)\,. \tag{1.15}$$

In a typical Monte Carlo calculation, tallies are made by adding some score, multiplied by the current particle weight, to an accumulator. To calculate a similar quantity related to the Monte Carlo particle density would be very close to calculating any other quantity but without including the particle weight. The goal of FW-CADIS is to make the Monte Carlo particle density, $m(\overrightarrow{r}, E)$, uniform over the tally areas, so an importance map must be developed that represents the importance of achieving uniform Monte Carlo particle density. By attempting to keep the Monte Carlo particle density more uniform, more uniform relative errors for the tallies should be realized.

Two options for forward weighting are possible. For tallies over some area where the entire group-wise flux is needed with low relative uncertainties, the adjoint source should be weighted inversely by the forward flux, $\phi(\overrightarrow{r}, E)$. The other option, for a tally in which only an energy-integrated quantity is desired, is to weight the adjoint inversely by that energy-integrated quantity, $\int \sigma_d(E)\,\phi(\overrightarrow{r}, E)$ dE. For a tally in which the total flux is desired, then the response in the adjoint source is simply $\sigma_d(E) = 1$.

To optimize the forward Monte Carlo simulation for the calculation of some quantity at multiple tally locations or across a mesh tally, the adjoint source must be weighted by the estimate of that quantity. For a tally defined by its spatial location $g(\overrightarrow{r})$ and its optional response $\sigma_d(E)$, the standard adjoint source would be $q^+(\overrightarrow{r}, E) = \sigma_d(E)\,\mathrm{g}(\overrightarrow{r})$. The forward-weighted adjoint source, $q^+(\overrightarrow{r}, E)$, depending on what quantity is to be optimized, is listed below.

For the calculation of		Adjoint source
Energy and spatially dependent flux	$\phi\left(\overrightarrow{r}, E\right)$	$\frac{g\left(\overrightarrow{r}\right)}{\phi\left(\overrightarrow{r}, E\right)}$
Spatially dependent total flux	$\int \phi\left(\overrightarrow{r}, E\right) dE$	$\frac{g\left(\overrightarrow{r}\right)}{\int \phi\left(\overrightarrow{r}, E\right) dE}$
Spatially dependent total response	$\int \sigma_d\left(E\right) \phi\left(\overrightarrow{r}, E\right) dE$	$\frac{\sigma_d\left(E\right) \mathrm{g}\left(\overrightarrow{r}\right)}{\int \sigma_d\left(E\right) \phi\left(\overrightarrow{r}, E\right) dE}$

The bottom line of FW-CADIS is that in order to calculate a quantity at multiple tally locations (or across a mesh tally) with more uniform relative uncertainties, an adjoint source must be developed for an objective function that keeps some non-physical quantity—related to the Monte Carlo particle density and similar in form to the desired quantity—constant. FW-CADIS uses the solution of a forward discrete-ordinates calculation to properly weight the adjoint source. After that, the standard CADIS approach is used.

1.2.5 MAVRIC Implementation of CADIS

With MAVRIC, as with other shielding codes, the user defines the problem as a set of physical models—the material compositions, the geometry, the source, and the detectors (locations and response functions)—as well as some mathematical parameters on how to solve the problem (number of histories, etc.). For the variance reduction portion of MAVRIC, the only additional inputs required are (1) the mesh planes to use in the discrete-ordinates calculation(s) and (2) the adjoint source description——basically the location and the response of each tally to optimize in the forward Monte Carlo calculation. MAVRIC uses this information to construct a Denovo adjoint problem. (The adjoint source is weighted by a Denovo forward flux or response estimate for FW-CADIS applications.) MAVRIC then uses the CADIS methodology: it combines the adjoint flux from the Denovo calculation with the source description and creates the importance map (weight window targets) and the mesh-based biased source. Monaco is then run using the CADIS biased source distribution and the weight window targets.

Denovo

Denovo is a parallel three-dimensional SN code that is used to generate adjoint (and, for FW-CADIS, forward) scalar fluxes for the CADIS methods in MAVRIC. For use in MAVRIC/CADIS, it is highly desirable that the SN code be fast, positive, and robust. The phase-space shape of the forward and adjoint fluxes, as opposed to a highly accurate solution, is the most important quality for Monte Carlo weight-window generation. Accordingly, Denovo provides a step-characteristics spatial differencing option that produces positive scalar fluxes as long as the source (volume plus in-scatter) is positive. Denovo uses an orthogonal, nonuniform mesh that is ideal for CADIS applications because of the speed and robustness of calculations on this mesh type.

Denovo uses the highly robust GMRES (Generalized Minimum Residual) Krylov method to solve the SN equations in each group. GMRES has been shown to be more robust and efficient than traditional source (fixed-point) iteration. The in-group discrete SN equations are defined as

$$\mathbf{L}\psi = \mathrm{MS}\phi + q \tag{1.16}$$

where $\mathbf{L}$ is the differential transport operator, $\mathbf{M}$ is the moment-to-discrete operator, $\mathbf{S}$ is the matrix of scattering cross section moments, q is the external and in-scatter source, ϕ is the vector of angular flux moments, and ψ is the vector of angular fluxes at discrete angles. Applying the operator $\mathbf{D}$, where $\phi = \mathbf{D}\psi$, and rearranging terms, casts the in-group equations in the form of a traditional linear system, $\mathbf{A}x = b$,

$$\left(\mathbf{I} - \mathbf{D}\mathbf{L}^{-1}\mathrm{MS}\right) = \mathbf{D}\mathbf{L}^{-1}q. \tag{1.17}$$

The operation $\mathbf{L}^{-1}\nu$, where ν is an iteration vector, is performed using a traditional wave-front solve (transport sweep). The parallel implementation of the Denovo wave-front solver uses the well-known Koch-Baker-Alcouffe (KBA) algorithm, which is a two-dimensional block-spatial decomposition of a three-dimensional orthogonal mesh [BK98]. The Trilinos package is used for the GMRES implementation [WH03] Denovo stores the mesh-based scalar fluxes in a double precision binary file (*.dff) called a *Denovo flux file*. Past versions of SCALE/Denovo used the TORT [RS97] *.varscl file format (DOORS package [RC98]), but this was limited to single precision. Since the rest of the MAVRIC sequence has not yet been parallelized, Denovo is currently used only in serial mode within MAVRIC.

Monaco

The forward Monte Carlo transport is performed using Monaco, a fixed-source shielding code that uses the SCALE General Geometry Package (SGGP, the same as used by the criticality code KENO-VI) and the standard SCALE material information processor. Monaco can use either MG or CE cross section libraries. Monaco was originally based on the MORSE Monte Carlo code but has been extensively modified to modernize the coding, incorporate more flexibility in terms of sources/tallies, and read a user-friendly block/keyword style input.

Much of the input to MAVRIC is the same as Monaco. More details can be found in the Monaco chapter of the SCALE manual (SECTIONREFERENCE).

Running MAVRIC

The objective of a SCALE sequence is to execute several codes, passing the output from one to the input of the next, in order to perform some analysis——tasks that users typically had to do in the past. MAVRIC does this for difficult shielding problems by running approximate discrete-ordinates calculations, constructing an importance map and biased source for one or more tallies that the user wants to optimize in the Monte Carlo calculation, and then using those in a forward Monaco Monte Carlo calculation. MAVRIC also prepares the forward and adjoint cross sections when needed. The steps of a MAVRIC sequence are listed in Table 1.1. The user can instruct MAVRIC to run this whole sequence of steps or just some subset of the steps to verify the intermediate steps or to reuse previously calculated quantities in a new analyses.

The MAVRIC sequence can be stopped after key points by using the "parm= *parameter* " operator on the "=mavric" command line, which is the first line of the input file. The various parameters are listed in Table Table 1.2. These parameters allow the user to perform checks and make changes to the importance map calculation before the actual Monte Carlo calculation in Monaco.

MAVRIC also allows the sequence to start at several different points. If an importance map and biased source have already been computed, they can then be used directly. If the adjoint scalar fluxes are known, they can quickly be used to create the importance map and biased source and then begin the forward Monte Carlo calculation. All of the different combinations of starting MAVRIC with some previously calculated quantities are listed in the following section detailing the input options.

When using MG cross section libraries that do not have flux-to-dose-rate conversion factors, use "parm=nodose" to prevent the cross section processing codes from trying to move these values into the working library.

MAVRIC creates many files that use the base problem name from the output file. For an output file called "c:path1path2*outputName*.out" or "/home/path1/path2/ *outputName*.inp", spaces in the output name will cause trouble and should not be used.

Table 1.1: Steps in the MAVRIC sequence

Cross section calculation	XSProc is used to calculate the forward cross sections for Monaco
Forward Denovo (optional)	
Cross section calculation	XSProc is used to calculate the forward cross sections for Denovo
Forward flux calculation	Denovo calculates the estimate of the forward flux
Adjoint Denovo (optional)	
Cross section calculation	XSProc is used to calculate the adjoint cross sections for Denovo
Adjoint flux calculation	Denovo calculates the estimate of the adjoint flux
CADIS (optional)	The scalar flux file from Denovo is then used to create the biased source distribution and transport weight windows
Monte Carlo calculation	Monaco uses the biased source distribution and transport weight windows to calculate the various tallies

Table 1.2: Parameters for the MAVRIC command line ("parm=...")

Parameter	MAVRIC will stop after
check	input checking
forinp	Forward Denovo input construction (makes `xkba_b.inp` in the tmp area)
forward	The forward Denovo calculation
adjinp	Adjoint Denovo input construction (makes `xkba_b.inp` in the tmp area)
adjoint	The adjoint Denovo calculation
impmap	Calculation of importance map and biased source

1.3 MAVRIC input

The input file for MAVRIC consists of three lines of text ("=mavric" command line with optional parameters, the problem title, and SCALE cross section library name) and then several blocks, with each block starting with "read xxxx" and ending with "end xxxx". There are three required blocks and nine optional blocks. Material and geometry blocks must be listed first and in the specified order. Other blocks may be listed in any order.

Blocks (must be in this order):

- Composition – (required) SCALE standard composition, list of materials used in the problem
- Celldata – SCALE resonance self-shielding
- Geometry – (required) SCALE general geometry description
- Array – optional addition to the above geometry description
- Volume – optional calculation or listing of region volumes
- Plot – create 2D slices of the SGGP geometry

Other Blocks (in any order, following the blocks listed above):

- Definitions – defines locations, response functions, and grid geometries used by other blocks
- Sources – (required) description of the particle source spatial, energy, and directional distributions

- Tallies – description of what to calculate: point detector tallies, region tallies, or mesh tallies
- Parameters – how to perform the simulation (random number seed, how many histories, etc.)
- Biasing – data for reducing the variance of the simulation
- ImportanceMap – instructions for creating an importance map based on a discrete-ordinates calculation

The material blocks (Composition and Celldata) and the physical model blocks (Geometry, Array, Volume, and Plot) follow the standard SCALE format. See the other SCALE references as noted in the following sections for details. The Biasing block and ImportanceMap block cannot both be used.

For the other six blocks, scalar variables are set by "keyword=value", fixed-length arrays are set with "keyword $value_1$ … $value_N$", variable-length arrays are set with "keyword $value_1$ … $value_N$ end", and some text and filenames are read in as quoted strings. Single keywords to set options are also used in some instances. The indention, comment lines, and upper/lowercase shown in this document are not required— they are used in the examples only for clarity. Except for strings in quotes (like filenames), SCALE is case insensitive.

After all input blocks are listed, a single line with "end data" should be listed. A final "end" should also be listed, to signify the end of all MAVRIC input. Nine of the blocks are the same input blocks as those used by the functional module Monaco, with a few extra keywords only for use with MAVRIC. These extra keywords are highlighted here, but without relisting all of the standard Monaco keywords for those blocks. See Table 1.3 for an overview of MAVRIC input file structure.

1.3.1 Composition block

Material information input follows the standard SCALE format for material input. Basic materials known to the SCALE library may be used as well as completely user-defined materials (using isotopes with known cross sections). Input instructions are located in the XSProc chapter (SECTIONREFERENCE) in the SCALE manual. The Standard Composition Library chapter (SECTIONREFERENCE) lists the different cross section libraries and the names of standard materials. An example is as follows:

```
read
 composition


u
o2 1 0
.2 293
.0 92234 0
.0055 92235 3
.5 92238 96
.4945 end


o
r
c
o
n
c
r
e
t
e 2 1
.0 293
.0 end
```

(continues on next page)

(continued from previous page)

```
s
s304 3 1
.0 293
.0 end

end
 composition
```

Details on the cell data block are also included in the XSProc chapter (SECTIONREFERENCE). When using different libraries for the importance map production (listed at the top of the input) and the final Monte Carlo calculation (listed in the parameters block, if different), make sure that the materials are present in both libraries.

Table 1.3: Overall input format

input file	Comment
=mavric	name of sequence
	title
S	cross section library name
o	SCALE material compositions
m	[required block]
e	
t	SCALE resonance self-shielding
i	[optional block]
t	
l	SCALE SGGP geometry
e	[required block]
f	
o	SCALE SGGP arrays
r	[optional block]
t	
h	SCALE SGGP volume calc
i	[optional block]
s	
p	SGGP Plots
r	[optional block]
o	
b	Definitions
l	[possibly required]
e	
m	Sources definition
	[required block]
v7	
-27	Tally specifications
n19	[optional block]
g	
read	Monte Carlo parameters
composition	[optional block]
.	Biasing information
.	[optional block]
.	
end	Importance map
composition	[optional block]
read	
celldata	end of all blocks
	end of MAVRIC input
.	
.	
.	
end	
celldata	
read	
geometry	
.	
.	
.	
end	
geometry	
read	
array	

.	
.	
.	
end	

1.3.2 SGGP geometry blocks

MAVRIC uses the functional module Monaco for the forward Monte Carlo calculation. Monaco tracks particles through the physical geometry described by the SGGP input blocks, as well as through the mesh importance map and any mesh tallies, which are defined in the global coordinates and overlay the physical geometry. Because Monaco must track through all of these geometries at the same time, users should not use the reflective boundary capability in the SGGP geometry.

For more details on each SGGP geometry block, see the following sections of the KENO-VI chapter (SECTIONREFERENCE) of the SCALE Manual.

Geometry – *Geometry Data*

Array – *Array Data*

Volume – *Volume Data*

Plot – *Plot Data*

1.3.3 Other blocks shared with Monaco

The definitions, sources, tallies, and biasing blocks are all the same as Monaco. They are all fully described in the Monaco chapter (SECTIONREFERENCE) of the SCALE Manual.

Definitions – *Definitions Block*

Sources – *Sources Block*

Tallies – *Tallies Block*

Biasing – *Biasing Block*

The parameters block includes several keywords that are not included in Monaco (see the *Parameter Block* section of the Monaco chapter (SECTIONREFERENCE)) which are used when the cross section library used in the importance calculations differs from the library used in the final forward Monaco Monte Carlo calculation. The library listed at the beginning of the MAVRIC input file will be used for the importance calculations (forward and adjoint Denovo calculation, formation of the importance map, and biased sources). To use a different MG library in the final Monaco simulation, use the keyword "library=" with the cross section library name in quotes. A cross section library for Monaco will be made using csas-mg. If there are any extra parameters to use ("parm=" in the "=csas-mg" line of the csas-mg input), they can be passed along using the keyword "parmString=" with the extra information in quotes. For example, the following input file would use a coarse-group library for the importance calculations and a fine-group library for the final Monaco, each with CENTRM processing.

```
=mavric parm=centrm

v7
-27
n19
g

...

read
 parameters


l
i
b
r
a
r
y
=
"
v7
-200
```

(continues on next page)

(continued from previous page)

```
...

end
 parameters


...

end
 data

end
```

To use a CE cross section in the final Monaco step, use the keyword "ceLibrary=" with the cross section library name in quotes. When the "library=" or "ceLibrary=" keywords are used, they should precede the "neutron", "photon", "noNeutron", and "noPhoton" keywords. Table 1.4 summarizes all of the keywords in the MAVRIC parameter block.

When using two different cross section libraries, be sure that the responses and distributions are defined in ways that do not depend on the cross section library. For example, any response that is just a list of n values (corresponding to a cross section library of n groups) needs to have the group energies specifically listed so that it can be evaluated properly on the other group structure.

Table 1.4: Extra keywords for the parameters block

block	keyword	type	length	default	required	restrictions/comments
read parameters						
	All of the keywords listed in the Monaco manual still apply					
	Final Monaco Monte Carlo calculation is multi-group					
	library=	character	not present		no	multi-group library for final Monaco run, if different than MAVRIC
	parmString=	character	not present		no	parm for MG cross section processing using CSAS-MG
	Final Monaco Monte Carlo calculation is continuous energy					
	ceLibrary=	character	not present		no	continuous energy library name
end parameters						

1.3.4 Importance map block

The importance map block is the "heart and soul" of MAVRIC. This block lists the parameters for creating an importance map and biased source from one (adjoint) or two (forward, followed by adjoint) Denovo discrete-ordinates calculations. Without an importance map block, MAVRIC can be used to run Monaco and use its conventional types of variance reduction. If both the importance map and biasing blocks are specified, then only the importance map block will be used. The various ways to use the importance map block are explained in the subsections below. Keywords for this block are summarized at the end of this section, in Table 1.5.

Constructing a mesh for the S_N calculation

All uses of the importance map block that run the discrete-ordinates code require the use of a grid geometry that overlays the physical geometry. Grid geometries are defined in the definitions block of the MAVRIC input. The extent and level of detail needed in a grid geometry are discussed in the following paragraphs.

When using S_N methods alone for solving radiation transport in shielding problems, a good rule of thumb is to use mesh cell sizes on the order of a meanfree path of the particle. In complex shielding problems, this could lead to an extremely large number of mesh cells, especially when considering the size of the meanfree path of the lowest energy neutrons and photons in common shielding materials.

In MAVRIC, the goal is to use the S_N calculation for a quick approximate solution. Accuracy is not paramount—just getting an idea of the overall shape of the true importance map will help accelerate the convergence of the forward Monte Carlo calculation. The more accurate the importance map, the better the forward Monte Carlo acceleration will be. At some point there is a time trade-off when the computational time for calculating the importance map followed by the time to perform the Monte Carlo calculation exceeds that of a standard analog Monte Carlo calculation. Large numbers of mesh cells that result from using very small mesh sizes for S_N calculations also use a great deal of computer memory.

Because the deterministic solution(s) for CADIS and FW-CADIS can have moderate fidelity and still provide variance reduction parameters that substantially accelerate the Monte Carlo solution, mesh cell sizes in MAVRIC applications can be larger than what most S_N practioners would typically use. The use of relatively coarse mesh reduces memory requirements and the run time of the deterministic solution(s). Some general guidelines to keep in mind when creating a mesh for the importance map/biased source are as follows:

- The true source regions should be included in the mesh with mesh planes at their boundaries.
- Place point or very small sources in the center of a mesh cell, not on the mesh planes.
- Any region of the geometry where particles could eventually contribute to the tallies (the "important" areas) should be included in the mesh.
- Point adjoint sources (corresponding to point detector locations) in standard CADIS calculations do not have to be included inside the mesh. For FW-CADIS, they must be in the mesh and should be located at a mesh cell center, not on any of the mesh planes.
- Volumetric adjoint sources should be included in the mesh with mesh planes at their boundaries.
- Mesh planes should be placed at significant material boundaries.
- Neighboring cell sizes should not be drastically different.
- Smaller cell sizes should be used where the adjoint flux is changing rapidly, such as toward the surfaces of adjoint sources and shields (rather than in their interiors).

Another aspect to keep in mind is that the source in the forward Monaco Monte Carlo calculation will be a biased mesh-based source. Source particles will be selected by first sampling which mesh cell to use and then sampling a position uniformly within that mesh cell that meets the user criteria of "unit=", "region=", or "mixture=" if specified. The mesh should have enough resolution that the mesh source will be an accurate representation of the true source.

The geometry for the Denovo calculation is specified using the keyword "gridGeometryID=" and the identification number of a grid geometry that was defined in the definitions block. The material assigned to each voxel of the mesh is determined by testing the center point in the SGGP geometry (unless the macro-material option is used—see below).

Macromaterials for S_N geometries

Part of the advantage of the CADIS method is that the adjoint discrete-ordinates calculation only needs to be approximate in order to form a reasonable importance map and biased source. This usually means that the mesh used is much coarser than the mesh that would be used if the problem were to be solved only with a discrete-ordinates code. This coarse mesh may miss significant details (especially curves) in the geometry and produce a less-than-optimal importance map.

To get more accurate solutions from a coarse-mesh discrete-ordinates calculation, Denovo can represent the material in each voxel of the mesh as a volume-weighted mixture of the real materials, called *macromaterials*, in the problem. When constructing the Denovo input, the Denovo EigenValue Calculation (DEVC, see section SECTIONREFERENCE) sequence can estimate the volume fraction occupied by using each real material in each voxel by a sampling method. The user can specify parameters for how to sample the geometry. Note that finer sampling makes more accurate estimates of the material fraction but requires more setup time to create the Denovo input. Users should understand how the macromaterials are sampled and should consider this when constructing a mesh grid. This is especially important for geometries that contain arrays. Careful consideration should be given when overlaying a mesh on a geometry that contains arrays of arrays.

Because the list of macromaterials could become large, the user can also specify a tolerance for how close two different macromaterials can be in order to be considered the same, thereby reducing the total number of macromaterials. The macromaterial tolerance, "`mmTolerance=`", is used for creating a different macromaterial from the those already created by looking at the infinity norm between two macromaterials. The number of macromaterials does not appreciably impact Denovo run time or memory requirements.

Two different sampling methods are available—point testing [IPE+09] with the keyword `mmPointTest` and ray tracing [Joh13] with the keyword `mmRayTest`.

Ray Tracing

This method estimates the volume of different materials in the Denovo mesh grid elements by tracing rays through the SGGP geometry and computing the average track lengths through each material. Rays are traced in all three dimensions to better estimate the volume fractions of materials within each voxel. The mmSubCell parameter controls how many rays will be traced in each voxel in each dimension. For example, if mmSubCell= n, then when tracing rays in the z dimension, each column of voxels uses a set of n×n rays starting uniformly spaced in the x and y dimensions. With rays being cast from all three orthogonal directions, a total of 3n2 rays are used to sample each voxel. One can think of subcells as an equally spaced sub-mesh with a single ray positioned at each center. The number of subcells in each direction, and hence the number of rays, can be explicitly given with mmSubCells ny nz nx nz nx ny end keyword for rays parallel to the x axis, y axis, and z axis. Fig. 1.1 shows different subcell configurations (in two dimensions) for a given voxel.

Ray tracing is a more robust method compared to the simple point testing method used in previous versions of SCALE/MAVRIC; however, it requires more memory than point testing. Ray tracing gives more accurate estimates of volume fractions because track lengths across a voxel give more information than a series of test points. Ray tracing is also much faster than point testing because the particle tracking routines are optimized to quickly determine lists of materials and distance along a given ray.

Ray tracing operates on the grid geometry supplied by the user and shoots rays in all three directions, starting from the lower bounds of the mesh grid. An example of an arbitrary assembly geometry is shown in Fig. 1.2. A ray consists of a number of steps that each correspond to crossing a material boundary along the path of the ray. Ratios of each step's length to the voxel length in the ray's direction determine the material volume fraction of that step in that voxel, and summation of the same material volume fractions gives the material volume fraction of that material in that voxel. Ray tracing through a single voxel that contains a fuel pin is illustrated in Fig. 1.3.

The final constructed macromaterials for this model are also shown in Fig. 1.2. Voxels that contain only a single material are assigned the original material number in the constructed macromaterials. For the voxels that contain a

Fig. 1.1: Ray positions within a voxel with different mmSubCells parameters.

Fig. 1.2: Geometry model (left) and the Denovo representation (right) of an assembly using macromaterials determined by ray tracing.

Fig. 1.3: Ray tracing (in two dimensions) through a voxel.

fuel pin with three different materials, the result is a new macromaterial consisting of the volume weighted fractions of each original material.

After the rays are shot in all three directions, the material volume fractions are updated, and macromaterials are created by using these material volume fractions. Material volume fraction calculations for a single voxel, as shown in Fig. 1.3, are given by

$$F_m = \sum_{d=x,y,z} \sum_{r=1}^{N_r} \sum_{s=1}^{N_s} \begin{cases} \frac{L_{d,r,s}}{L_d}, & m_s = m \\ 0, & \text{otherwise} \end{cases} \qquad and \qquad V_m = \frac{F_m}{\sum_{n=1}^{N_m} F_n}\ , \tag{1.18}$$

where *Fm* = sampled fraction of material *m* in the voxel,

d = direction of the rays (*x, y, z*),

r = ray number,

N_r = total number of rays in the voxel for direction of *d*,

s = step number,

N_s = total number of steps for ray r in the voxel for direction of *d*,

$L_{d,r,s}$ = length of the steps s for ray r in the voxel for direction of *d*,

L_d = length of the voxel along direction of *d*,

m_s = material of step *s*,

m = material number,

N_m = total number of materials in the voxel, and

V_m = volume fraction of material m in the voxel.

Point Testing

The recursive bisection method is utilized in point testing and uses a series of point tests to determine the macromaterial fractions. For a given voxel, the material at the center is compared to the material at the eight corners. If they are all the same, then the entire volume is considered to be made of that material. If they are different, then the volume is divided into two in each dimension. Each subvolume is tested, and the method is then applied to the subvolumes that are not of a single material. When the ratio of the volume of the tested region to the original voxel becomes less than a user-specified tolerance (in the range of 10-1 to 10-4), then further subdivision and testing are stopped. This is illustrated in Fig. **??**.

Fig. 4 Successive steps in the recursive macromaterial method

In point testing, the keyword "mmTolerance=f" is interpreted to be where *f* is the smallest fraction of the voxel volume that can be achieved by bisection method and hence the limiting factor for dividing the voxel. This same tolerance *f* is also used to limit the number of macromaterials. Before a new macromaterial is created, if one already exists where the fraction of each actual material matches to within the given tolerance, then the existing material will be used. If using only a single point at the center of each voxel, then use "mmTolerance=1". The mmSubCell keyword is not used in point testing.

Example

Fig. 1.4 shows an example of a cask geometry with two types of spent fuel (yellows), steel (blue), resin (green), and other metals (gray). When the Denovo geometry is set up by testing only the center of each mesh cell, the curved surfaces are not well represented (upper right). By applying the ray-tracing method and defining a new material made of partial fractions of the original materials, an improved Denovo model can be made. In the lower left of the figure, the Denovo model was constructed using one ray (in each dimension) per voxel and a tolerance of 0.1. This gives 20 new materials that are a mixture of the original 13 actual materials and void. With mmSubCells=3 and an mmTolerance=0.01, 139 macromaterials are created.

A macromaterial table listing the fractions of each macromaterial is saved to a file called "outputName.mmt", where outputName is the name the user chose for his or her output file. This file can be used by the Mesh File Viewer to display the macromaterials as mixtures of the actual materials, as seen in the lower row of Fig. 1.4. See the Mesh File Viewer help pages for more information on how to use colormap files and macromaterial tables.

Optimizing source/detector problems

For standard source/detector problems in which one tally is to be optimized in the forward Monte Carlo calculation, an adjoint source based on that tally must be constructed. An adjoint source requires a unique and positive identification number, a physical location, and an energy spectrum. The adjoint source location can be specified either by (1) a point location ("locationID=" keyword) or (2) a volume described by a box ("boundingBox" array). A bounding box is specified by maximum and minimum extent in each dimension—x_{max} x_{min} y_{max} y_{min} z_{max} z_{min}—in global coordinates. The boundingBox should not be degenerate (should have volume>0) but can be optionally limited to areas matching a given unit number ("unit="), a given region number ("region="), or a given material mixture number ("mixture="). A mixture and a region cannot both be specified, since that would either be redundant or mutually exclusive. The energy spectrum of an adjoint source is a response function ("responseID=") listing one of the ID numbers of the responses defined in the definitions block. An optional weight can be assigned to each adjoint source using the "weight=" keyword. If not given, the default weight is 1.0.

For example, to optimize a region tally, the user would construct an adjoint source located in the same place as the tally, with an adjoint source spectrum equal to the response function that the tally is computing. Note that the grid geometry 1 and response function 3 must already be defined in the definitions block.

Fig. 1.4: Cask geometry model (upper left) and the Denovo representation using cell center testing (upper right). Representations using macromaterials determined by ray tracing are shown for mmSubCell=1/mmTolerance=0.1 (lower left) and mmSubCell=3/mmTolerance=0.01 (lower right).*

```
read
 importanceMap

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=1

a
d
j
o
i
n
t
S
o
u
r
c
e 24

b
o
u
n
d
i
n
g
B
o
x 12
.0 10
.0  5
.0
-5
.0  10
.0
-10
.0

u
n
i
t
=1
```

(continues on next page)

```
r
e
g
i
o
n
=5
```

(continued from previous page)

```
r
e
s
p
o
n
s
e
I
D
=3
   end
 adjointSource
end
 importanceMap
```

For optimizing a point detector for the calculation of total photon flux, the importance map block would look like the following:

```
read
 importanceMap

a
d
j
o
i
n
t
S
o
u
r
c
e 21

l
o
c
a
t
i
o
n
I
D
=4

r
e
s
p
o
n
s
e
I
D
=1
```

(continues on next page)

(continued from previous page)

```
   end
 adjointSource

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=1
end
 importanceMap
```

where location 4 is the same location used by the point detector. To calculate total photon flux, response function 1 must be defined in the definitions block similar to this response:

```
read
 definitions

r
e
s
p
o
n
s
e 1

v
a
l
u
e
s 27
r0
.0 19
r1
. end
    end
 response

...
end
 definitions
```

This response is used for computing total photon flux for the 27 neutron/19 photon group coupled cross section library or like this response

```
read
 definitions

r
e
s
p
o
n
s
e 1

p
h
o
t
o
n

b
o
u
n
d
s 1000
.0 2
.0
e7 end

v
a
l
u
e
s  1
.0   1
.0   end
    end
 response

...
end
 definitions
```

which is independent of the cross section library.

Multiple adjoint sources

If there are several tallies in very close proximity and/or several different responses being calculated by the tallies, multiple adjoint sources can be used.

```
read
 importanceMap

g
r
i
```

(continues on next page)

```
d
G
o
m
e
t
```

(continued from previous page)

```
a
d
j
o
i
n
t
S
o
u
r
c
e 1

l
o
c
a
t
i
o
n
I
D
=4
r
e
s
p
o
n
s
e
I
D
=20
   end
 adjointSource

a
d
j
o
i
n
t
S
o
u
r
c
e 2

l
o
c
```

(continues on next page)

```
a
t
i
o
n
I
D
=5
```

(continued from previous page)

```
w
e
i
g
h
t
=2
.0
   end
 adjointSource
end
 importanceMap
```

Note that adjoint sources using point locations can be mixed with volumetric adjoint sources (using bounding boxes).

Options for Denovo S_n calculations

While the default values for various calculational parameters and settings used by Denovo for the MAVRIC sequence should cover most applications, they can be changed if desired. The two most basic parameters are the quadrature set used for the discrete ordinates and the order of the Legendre polynomials used in describing the angular scattering. The default quadrature order that MAVRIC uses is a level symmetric S_8 set, and the default scattering order is P_3 (or the maximum number of coefficients contained in the cross-section library if less than 3). S_8/ P_3 is an adequate choice for many applications, but the user is free to changes these. For complex ducts or transport over large distances at small angles, S_{12} may be required. S_4/ P_1 or even S_2/ P_0 would be useful in doing a very cursory run to confirm that the problem was input correctly, but this would likely be inadequate for weight window generation in a problem that is complex enough to require advanced variance reduction.

These and other Denovo options are applied to both the forward and the adjoint calculations that are required from the inputs given in the importance map block.

In problems with small sources or media that are not highly scattering, discrete ordinates can suffer from "ray effects" [Lat68][Lat71] where artifacts of the discrete quadrature directions can be seen in the computed fluxes. Denovo has a first-collision capability to help alleviate ray effects. This method computes the uncollided flux in each mesh cell from a point source. The uncollided fluxes are then used as a distributed source in the main discrete-ordinates solution. At the end of the main calculation, the uncollided fluxes are added to the fluxes computed with the first collision source, forming the total flux. While this helps reduce ray effects in many problems, the first-collision capability can take a significant amount of time to compute on a mesh with many cells or for many point sources.

Adjoint sources that use point locations will automatically use the Denovo first-collision capability. Volumetric adjoint sources (that use a boundingBox) will be treated without the first-collision capability. The keywords "firstCollision" and "noFirstCollision" will be ignored by MAVRIC for adjoint calculations. Keywords for Denovo options in the importance map block are summarized at the end of this section, in Table 1.6.

Starting with an existing adjoint flux file

An importance map can be made from an existing Denovo flux file by using the keyword "adjointFluxes=" with the appropriate file name in quotes. The file must be a binary file using the *.dff file format, and the number of groups must match the number of groups in the MAVRIC cross section library (i.e., the library entered on the third line of the MAVRIC input file). Instead of performing an adjoint calculation, the fluxes read from the file will be used to create both the mesh-based importance map and the biased mesh source.

```
read
 importanceMap

a
d
j
o
i
n
t
F
l
u
x
e
s
=
"
c
:
\
m
y
d
o
c
u
~1
\
p
r
e
v
i
o
u
s
R
u
n
.
a
d
j
o
i
n
t
.
d
f
f
"
```

(continues on next page)

(continued from previous page)

```
g
r
i
d
G
e
o
m
e
t
r
y
=7
end
 importanceMap
```

If the "adjointFluxes=" keyword is used and any adjoint sources are defined, an error will result. If a forward flux file is supplied for forward-weighting the adjoint source (see below), then an adjoint flux file cannot be specified.

The grid geometry is not required when using a pre-existing flux file. If grid geometry is not supplied, one will be created from the mesh planes that are contained in the Denovo flux file (which were used to compute the fluxes in that file).

Forward-weighting the adjoint source

To optimize a mesh tally or multiple region tallies/point detector tallies over a large region, instead of a uniform weighting of the adjoint source, a weighting based on the inverse of the forward response can be performed. This requires an extra discrete-ordinates calculation but can help the forward Monte Carlo calculation compute the mesh tally or group of tallies with more uniform statistical uncertainties.

The same grid geometry will be used in both the forward calculation and the adjoint calculation, so the user must ensure that the mesh covers all of the forward sources and all of the adjoint sources, even if they are point sources.

To use forward-weighted CADIS, specify either of the keywords – "respWeighting" or "fluxWeighting". For either, MAVRIC will run Denovo to create an estimate of the forward flux, $\phi\left(\overrightarrow{r}, E\right)$. For response weighting ("respWeighting"), each adjoint source is inversely weighted by the integral of the product of the response function used in that adjoint source and the estimate of the forward flux. For an adjoint source described by the geometric function $g(\overrightarrow{r})$ and the response function $\sigma_d\left(E\right)$ (note that $\sigma_d\left(E\right) = 1$ for computing total fluxes), the forward-weighted adjoint source becomes

$$q_i^+\left(\overrightarrow{r}, E\right) = \frac{\sigma_d\left(E\right) g(\overrightarrow{r})}{\int \sigma_d\left(E\right)\ \phi\left(\overrightarrow{r}, E\right) \mathrm{dE}} \ . \tag{1.19}$$

Response weighting will calculate more uniform relative uncertainties of the integral quantities of the tallies in the final Monte Carlo calculation.

To optimize the calculation of the entire group-wise flux with more uniform relative uncertainties in each group, the adjoint source should be weighted inversely by the forward flux, $\phi\left(\overrightarrow{r}, E\right)$, using the "fluxWeighting" keyword. For an adjoint source described by the geometric function $g(\overrightarrow{r})$ and the response function $\sigma_d\left(E\right) = 1$, the forward-weighted adjoint source becomes

$$q_i^+\left(\overrightarrow{r}, E\right) = \frac{\sigma_d\left(E\right) g(\overrightarrow{r})}{\phi\left(\overrightarrow{r}, E\right)} \ . \tag{1.20}$$

For example, consider a problem with a single source and two detectors, one near the source that measures flux and one far from the source that measures some response. In a standard Monte Carlo calculation, it is expected that since

more Monte Carlo particles cross the near detector, it will have a much lower relative uncertainty than the far detector. Standard CADIS could be used to optimize the calculation of each in separate simulations:

To optimize the flux in the near detector	To optimize the response in the far detector
read importanceMap gridGeometryID=1 adjointSource 1 boundingBoxx1x2y1y2z1z2 responseID=1	read importanceMap gridGeometryID=1 adjointSource 2 boundingBoxu1u2v1v2w1w2 responseID=6

where response 1 was defined as $\sigma_1(E) = 1$ and response 6 was defined as $\sigma_6(E) =$ flux-to-response conversion factors. The two options for forward weighting allow the tallies for both detectors to be calculated in the same MAVRIC simulation. Using "fluxWeighting", the importance map and biased source will be made to help distribute Monte Carlo particles evenly through each energy group and every voxel in both detectors, making the relative uncertainties close to uniform. With "respWeighting", the importance map and biased source will optimize the total integrated response of each tally.

To optimize $\phi(\overrightarrow{r}, E)$ in each detector	To optimize a total response $\int \sigma_d(E)\,\phi(\overrightarrow{r}, E)dE$ (either total flux or total dose)
read importanceMap gridGeometryID=1 `nearDetector addjoinSource 1 boundingBox x1 x2 y1	read importanceMap gridGeometryID=1 `nearDetector addjoinSource 1 boundingBox x1 x2 y1

Using flux weighting, the adjoint source will be

$$q^{+}\left(\overrightarrow{r},E\right)=\frac{\sigma_{1}\left(E\right)g_{\text{near}}(\overrightarrow{r})}{\phi\left(\overrightarrow{r},E\right)}+\frac{\sigma_{6}\left(E\right)g_{\text{far}}(\overrightarrow{r})}{\phi\left(\overrightarrow{r},E\right)}\,, \tag{1.21}$$

or using response weighting, the adjoint source will be

$$q^{+}\left(\overrightarrow{r},E\right)=\frac{\sigma_{1}\left(E\right)g_{1}(\overrightarrow{r})}{\int\sigma_{1}\left(E\right)\phi\left(\overrightarrow{r},E\right)dE}+\frac{\sigma_{6}\left(E\right)g_{2}(\overrightarrow{r})}{\int\sigma_{6}\left(E\right)\phi\left(\overrightarrow{r},E\right)dE}\,. \tag{1.22}$$

This implementation is slightly different from the original MAVRIC in SCALE 6. The current approach is simpler for the user and allows the importance parameters to optimize the final Monte Carlo calculation for the calculation of two different responses in two different areas.

If the number of mesh cells containing the true source is less than 10, then MAVRIC will convert these source voxels to point sources and Denovo will automatically use its first-collision capability to help reduce ray effects in the forward calculation. The user can easily override the MAVRIC defaults—to force the calculation of a first-collision source no matter how many voxels contain source; this can be done by using the keyword "firstCollision". To prevent the calculation of a first-collision source, the keyword "noFirstCollision" can be used. If the keywords "firstCollision" or "noFirstCollision" are used, then they will only apply to the forward calculation, not the subsequent adjoint calculation.

The keyword "saveExtraMaps" will save extra files that can be viewed by the Mesh File Viewer. The source used by the forward Denovo calculation is stored in "*outputName*.dofs.3dmap", where *outputName* is the name the user chose for his output file.

Forward weighting with an existing forward flux file

Similar to the capability of using pre-existing adjoint flux files, MAVRIC can use a pre-existing forward flux file to create a forward-weighted adjoint source without performing the forward Denovo calculation. The user may specify the *.dff file containing the forward fluxes using the keyword "forwardFluxes=". The filename should be enclosed in quotes, and the file must be a binary file using the Denovo flux file format. The number of groups must match the number of groups in the MAVRIC cross section library (i.e., the library entered on the third line of the MAVRIC input file).

```
read
 importanceMap

f
o
r
w
a
r
d
F
l
u
x
e
s
=
"
c
:
\
m
y
a
o
c
u
```

(continues on next page)

(continued from previous page)

```
g
r
i
d
G
e
o
m
e
t
r
y
=7

a
d
j
o
i
n
t
S
o
u
r
c
e 1

.
.
.
     end
 adjointSource

r
e
s
p
W
e
i
g
h
t
i
n
g
end
 importanceMap
```

When using a pre-existing forward flux file, either “respWeighting” or “fluxWeighting” must still be specified.

Using the importance map

An importance map produced by the importance map block consists of the target weight values as a function of position and energy. The upper weight window used for splitting and the lower weight window used for Russian roulette are set by the window ratio. The window ratio is simply the ratio of the weight window's upper bound to the weight window lower bound, with the target weight being the average of the upper and lower bounds.

The keyword "windowRatio=" can be used within the importance map block to specify what window ratio will be used with the importance map that is passed to the Monaco forward Monte Carlo calculation. For a windowRatio of r, the upper weights for splitting, w_{max}, and the lower weights for Russian roulette, w_{min}, are set as

$$w_{\min} = \frac{2}{r+1}\overline{w} \tag{1.23}$$

and

$$w_{\max} = \frac{2r}{r+1}\overline{w} \tag{1.24}$$

for the target weight $\overline{w}$ in each mesh cell and for each energy of the importance map. The default value for the windowRatio is 5.0.

Other notes on importance map calculations

Since the importance map calculations all take place using mesh geometry, one of the first steps that occurs is to create a mesh representation of the true source (the forward source) on the same grid. This procedure uses the same two methods as the Monaco mesh source saver routine. Mesh cells can be subdivided and tested to see if they are within the defined source, or a set number of points can be sampled from the source. The keywords "subCells=" and "sourceTrials=" are used in the importance map block to change the default settings for constructing the mesh representation of the forward source.

If macromaterials are used ("mmTolerance<1") and the adjoint source is limited to a particular material, then the amount of adjoint source in a mesh voxel will be weighted by the material amount in that voxel.

In SCALE/MAVRIC, Denovo is called as a fixed-source S_N solver and cannot model multiplying media. Neither forward nor adjoint neutron calculations from Denovo will be accurate when neutron multiplication is a major source component. If neutron multiplication is not turned off in the parameters block of the MAVRIC input (using "fissionMult=0"), a warning will be generated to remind the user of this limitation.

By default, MAVRIC instructs Denovo not to perform outer iterations for neutron problems if the cross section library contains upscatter groups. This is because the time required calculating the fluxes using upscatter can be significantly longer than without. For problems in which thermal neutrons are an important part of the transport or tallies, the user should specify the keyword "upScatter=1" in the importance map block. This will instruct Denovo to perform the outer iterations for the upscatter groups, giving more accurate results but taking a much longer time for the discrete-ordinates calculation.

When performing a MAVRIC calculation using a coarse-group energy structure for Denovo (for example with the 27/19 library) but a fine-group energy structure (with the 200/47 library) for the final Monaco calculation, the source biasing parameters are determined on the coarse-group structure. The importance map (*.mim) file and the biased mesh source (*.msm) files all use the coarse-group structure. The source biasing information is then applied to fine-group mesh versions of the sources, resulting in the *.sampling.*.msm files. This way, the biased sources used in the final Monaco calculation retain their fine-group resolution. This can be especially important in representing the high-energy portion of the fission neutron distribution for example. When using CE-Monaco, the source sampling routines first use the *.msm files to determine the source particle's voxel and energy group. From that voxel and energy group, the user-given source distributions are used to sample the specific starting location and specific energy of the source particle. This way, the CE-Monaco calculation samples the true CE distributions.

Table 1.5: Keywords for the importance map block

block	keyword	type	length	default	required	restrictions/comments
importanceMap						
Perform an adjoint S_N calculation using one (or more) adjoint source(s) and a gridGeometry						
	gridGeometryID=	integer			yes	matches one of the id numbers from gridGeometries
	adjointSource id	integer			yes	non-negative integer, unique among adjointSources
	locationID=	integer			a*	matches one of the id numbers from locations
	boundingBox	real	6		b*	parameters: x_{max} x_{min} y_{max} y_{min} z_{max} z_{min}
						*required: either a) locationID= or b) boundingBox
	responseID=	integer			c*	single id number from responses
	responseIDs	integer	any	none	d*	list of id numbers from responses
						*required: either c) responseID= or d) responseIDs
	weight=	real		1.0	no	positive real number
	unit=	integer		-1	no	limit adjoint source in boundingBox to a unit
	region=	integer		-1	no	limit adjoint source in boundingBox to a region of a unit
	mixture=	integer		-1	no	limit adjoint source in boundingBox to a mixture
	end adjointSource					
Constructing the Denovo geometry using macro materials						
	macromaterial					
	mmSubCell=	integer		1	no	rays per dimension to throw at each voxel
	mmTolerance=	real		0.01	no	smallest volume fraction for macromaterial
	mmSubCells	integer	6		no	rays per dimension to throw (x:ny,nz; y:nx,nz; z: nx,ny)
	mmPointTest				no	use recursive bisection point testing method
	mmRayTest				no	use ray tracing method
	mmRTSpeed				no	optimize ray-tracing method for speed
	mmRTMemory				no	optimize ray-tracing method for memory conservation
	end macromaterial					
Constructing the mesh version of the true source						
	subCells=	integer		2	no	subcells per cell (each dimension)
	sourceTrials=	integer		1000000	no	how many source particles to sample
	reduce			not present	no	store the smallest cuboid around the voxels with source
Perform a forward S_N calculation and weight the adjoint source						
	fluxWeighting			not present	no	weight adjoint source with forward flux
	respWeighting			not present	no	weight adjoint source with integrated forward response
	saveExtraMaps			not present	no	save extra 3dmap files associated with forward calculation
	firstCollision			not present	no	forces the use a a first collision source
	noFirstCollision			not present	no	does not allow the use of a first collision source
Use existing forward flux file for weighting the adjoint source						
	forwardFluxes=	string		not present	no	legal file name for current system, in quotes
Use existing adjoint flux file to create importance map						
	adjointFluxes=	string		not present	no	legal file name for current system, in quotes
While using the importance map						
	windowRatio=	real		5.0	no	real number greater than one
	mapMultiplier=	real		1.0	no	multiply targetWeights in imp. Map
end importanceMap						

Table 1.6: Denovo options for the importance map block

block	keyword	type	length	default	required	restrictions/comments
importanceMap						
	Optional Denovo S_N code parameters					
	discretization=	integer		4	no	0-diamond-difference, 1-diamond-difference with flux fix-up:lin0, 2-theta-weighted diamond-difference, 3-linear-discontinuous finite element, 4-step characteristics, 5-trilinear discontinuous finite elem
	quadType=	integer		0	no	0-level symmetric, 1-Gauss-Legendre product, 2-QR
	legendre=	integer		3*	no	P_L, L=highest Legendre polynomial, L=0,1,2,3,… *default is to use min(the highest available in the data,3)
	tportcorrection=	integer		1*	no	transport correction: 0-none, 1-diagonal, 2-Cesaro *For P_2 or higher, the default is 2 (Cesaro)
	upScatter=	integer		0	no	upscatter iterations: 0-none, 1-yes, 2-ignore
	xblocks=	integer		1	no	parallel stuff
	yblocks=	integer		1	no	parallel stuff
	zblocks=	integer		1	no	parallel stuff
	numSets=	integer		1	no	?
	partUpscatter=	integer		1	no	partition upscatter (0-no, 1-yes)
	quadrature=	integer		8	no	level symmetric S_N quadrature, N=2, 4, 6, 8, 10, 12, 14, 16
	polarsPerOct=	integer		0	no	Gauss-Legendre product quadrature or QR
	azimuthsPerOct=	integer		0	no	Gauss-Legendre product quadrature or QR
	maxIters=	integer		20	no	maximum number of iterations
	diagnostics=	integer		0	no	0-no diganostics, 1-all diagnostics
	output=	integer		0	no	0-no ouput, 1-all output
	krylovSpaceSize=	integer		10	no	size in memory for Krylov space
	tolerance=	double		1.E-03	no	tolerance used in convergence test
	krylovType=	integer		0	no	0-GMRES, 1-BiCGStab
	eigenSolver=	integer		0	no	0-power iteration, 1-Arnoldi, 2-shifted inverse
	multiGSolover=	integer		0	no	0-Gauss-Seidel, 1-Krylov
	withinGSolver=	integer		0	no	0-Krylov, 1-residual Krylov, 2-source iteration
	mgSettings=	integer		1	no	0-user supplied, 1-automatic
	upGroupSolver=	integer		0	no	0-same as within-group solver, 1-Krylov, 2-residual Krylov, 3-source iteration, 4-single source iteration
	acceleration=	integer		0	no	0-none, 1-two grid
	maxItersMG=	integer		20	no	maximum number of iterations
	toleranceMG=	double		0.001	no	tolerance used in convergence test
end importanceMap						

1.4 MAVRIC output

1.4.1 Main text output file

Similar to other SCALE sequences, MAVRIC returns a text output file containing the output from the SCALE driver, the sequence itself, and all of the functional modules called. The SCALE driver output first displays the problem input file, and then the first reading of the input file by the MAVRIC sequence is shown (which includes some material processing information). If there are any errors or warnings about the input file, they will be shown next. Next in the output file are the different passes through the MAVRIC sequence—up to 10 parts. If any errors or warning messages (such as lack of memory) are generated during processing, they will be displayed here. Finally, the output files from each functional module are concatenated to the above output and shows the files returned to the user.

First, the Monaco section of output first reviews the input it received. First the geometry is reviewed, showing which materials are used in each region and the volume of that region, if input or calculated. Then a detailed list of other Monaco input is reviewed: cross section parameters, data definitions, the source description, the tallies, the Monte Carlo parameters, and the biasing parameters. For MAVRIC calculations, if an importance map is used, then its summary is also given. The "Mesh Importance Map Characterization" shows where the importance map may be changing too rapidly and may require more refinement.

For each Monaco batch, the output file lists the batch time and the starting random number for the next batch, which may be useful in rerunning only a portion of a problem. Once all of the batches are completed, a list of the various tally files that have been created is given. Finally, the tallies are summarized in a section entitled "Final Tally Results Summary." For each point detector, the total neutron and photon fluxes (uncollided and total) are given as well as the final response values for each response function. For each region tally, the total neutron and photon fluxes (both track-length and collision density estimates) are listed, followed by the final response values for each response function. Group-by-group details are saved to separate files for each tally.

1.4.2 Additional output files

In addition to the generous amount of data contained in the MAVRIC text output file, many other files are created containing the intermediate data used by the sequence and the final tally data. Many of the files produced can be viewed using the Mesh File Viewer or the Interactive Plotter capabilities of Fulcrum, which is distributed with SCALE. (Note that most of the images in this document were taken from the Mesh File Viewer from SCALE 6.1.) Table 1.7 lists the other output files, based on the name of the main output file (here called *outputName)*, that are available to the user. These files will be copied back to the directory where the input file was located. Many of the files come from Monaco and are discussed in the Monaco chapter of the SCALE manual (SECTIONREFERENCE).

Other files that the user may be interested in are listed in Table 1.8. These files are kept in the temporary directory where SCALE executes and are not copied back to the directory where the input file was located, unless specifically requested using a SCALE "`shell`" command. Curious users may also be interested in viewing the various input files (i_*) that the MAVRIC sequence writes in order to run the SCALE functional modules.

Table 1.7: Output files that are copied back to user's area when the sequence finishes[a]

Filename	Viewer	Description
Output Summary		
outputName.out		main text output file, contains results summary
Diagnostic files		
outputName.respid.chart	P	response input and MG representation for response *id*
outputName.gridid.3dmap	V	mesh version of geometry using grid geometry *id*
outputName.cylid.3dmap	V	mesh version of geometry using cylindrical geometry *id*
outputName.distid.chart	P	distribution input and sampling test for distribution *id*
Mesh Source Saver		
filename.msm	V	mesh representation of a single source or total source
filename.id.msm	V	mesh representation of multiple sources
filename.sampling.msm	V	biased representation of a single source or total source
filename.sampling.id.msm	V	biased representation of multiple sources
Importance Map Generation		
outputName.geometry.3dmap	V	voxelized geometry (cell-center testing only)
outputName.forward.dff	V	scalar forward flux estimate, $\phi\left(x,y,z,E\right)$
outputName.adjoint.dff	V	scalar adjoint flux estimate, $\phi^{+}\left(x,y,z,E\right)$
outputName.mim	V	Monaco mesh importance map, $\overline{w}\left(x,y,z,E\right)$
outputName.msm	V	Monaco mesh source, $\widehat{q}\left(x,y,z,E\right)$
outputName.mmt	V	macro-material table
Tally Files		
outputName.pdid.txt		detailed results for point detector tally *id*
outputName.pdid.chart	P	batch convergence data for point detector tally *id*

continues on next page

Table 1.7 – continued from previous page

Filename	Viewer	Description
outputName.rtid.txt		detailed results for region tally *id*
outputName.rtid.chart	P	batch convergence data for region tally *id*
outputName.mtid.3dmap	V	mesh tally for meshTally *id*
outputName.mtid.respxx.3dmap	V	mesh tally of response by group for meshTally *id* response xx
outputName.mtid.flux.txt		detailed results for the group-wise flux of meshTally *id*
outputName.mtid.tfluxtxt		detailed results for total flux of meshTally *id*
outputName.mtid.respxx.txt		detailed results for response xx of meshTally *id*

[a] V – can be displayed with the Mesh File Viewer capabilities of Fulcrum. *P* – can be displayed with the 2D plotting capabilities of Fulcrum.

Table 1.8: Other intermediate files—available in the temporary directory (may be useful for testing and debugging)

File-name	**Description**
ft02f001	AMPX formatted cross sections for Denovo
fort.51	text file, listings of the mixing table for Monaco
fort.52	text file, review of MAVRIC sequence input variables
fort.54	energy bin boundaries for the current cross section library
xkba_b.inp	binary input file for Denovo – rename to have a *.dsi extension (Denovo simple input) to be viewed via Mesh File Viewer

1.5 Sample problems

1.5.1 Graphite shielding measurements with CADIS

As shown in the Monaco sample problem for simulating the Ueki shielding experiments (Monaco chapter Graphite Shielding Measurements) (SECTIONREFERENCE), as the amount of shielding material between a source and detector increases, the time required to reach a certain level of relative uncertainty increases quickly. This example will use the MAVRIC automated variance reduction capability to optimize the calculation of the dose rate at the detector location by specifying an importance map block with an adjoint source made from the detector response function and the detector location.

Input file

The following is a listing of the file `mavric.graphiteCADIS.inp` located in the SCALE `samples\input` directory. This calculation will use the coarse-group shielding library (27n19g) for all of the importance map calculations and the fine-group library (200n47g) for the final Monaco step. Additions, compared to the file `monaco.graphite.inp`, include a grid geometry for the Denovo computational mesh, a mesh tally to better visualize the particle flow, and the importance map block to optimize the Monte Carlo calculation of the point detector.

```
=mavric

M
o
n
a
c
o
/
M
A
V
R
I
```

(continues on next page)

(continued from previous page)

```
v7
-27
n19
g

'-------------------------------------------------------------------------------
' Composition Block - standard SCALE input
'-------------------------------------------------------------------------------
read
 composition

p
a
r
a
(
h2
o
)    1          1
.0 293
.0 end

c
a
r
b
o
n       2
d
e
n
=1
.7 1
.0 300
.0 end
end
 composition

'-------------------------------------------------------------------------------
' Geometry Block - SCALE standard geometry package (SGGP)
'-------------------------------------------------------------------------------
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

c
u
b
o
i
d  1   25
.0
-25
```

(continues on next page)

(continued from previous page)

```
c
o
n
e    2  10
.35948  25
.01   0
.0 0
.0
r
o
t
a
t
e
a1
=
-90
a2
=
-90
a3
=0

c
u
b
o
i
d  3   90
.0  70
.0  40
.0
-40
.0   40
.0
-40
.0

c
u
b
o
i
d 99  120
.0
-30
.0  50
.0
-50
.0   50
.0
-50
.0

m
e
d
i
a 1 1  1
2
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a 0 1  2

m
e
d
i
a 2 1  3

m
e
d
i
a 0 1  99
-1
-2
-3

b
o
u
n
d
a
r
y 99
end
 geometry

'-------------------------------------------------------------------------------
' Definitions Block
'-------------------------------------------------------------------------------
read
 definitions

l
o
c
a
t
i
o
n 1

p
o
s
i
t
i
o
n 110 0 0
    end
 location
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e 5

t
i
t
l
e
="ANSI standard (1977) neutron flux-to-dose-rate factors"

s
p
e
c
i
a
l
D
o
s
e
=9029
    end
 response

d
i
s
t
r
i
b
u
t
i
o
n 1

t
i
t
l
e
="Cf-252 neutrons, Watt spectrum a=1.025 MeV and b=2.926/MeV"

s
p
e
c
i
a
l
=
```

(continues on next page)

(continued from previous page)

```
p
a
r
a
m
e
t
e
r
s 1
.025 2
.926 end
    end
 distribution

g
r
i
d
G
e
o
m
e
t
r
y 7

t
i
t
l
e
="large meshes in paraffin, 5 cm mesh for shield thicknesses"

x
L
i
n
e
a
r 5
-25 25

x
L
i
n
e
a
r 12 30 90

x
p
l
a
n
e
s 100 110 120
-30 end
```

(continues on next page)

(continued from previous page)

```
y
p
l
a
n
e
s
-50
-40 40 50 end

y
L
i
n
e
a
r 7
-35 35

z
p
l
a
n
e
s
-50
-40 40 50 end

z
L
i
n
e
a
r 7
-35 35
    end
 gridGeometry
end
 definitions

'------------------------------------------------------------------------------
' Sources Block
'   Cf-252 neutrons, Watt fission spectrum model
'   with a=1.025 MeV and  b=2.926/MeV
'------------------------------------------------------------------------------
read
 sources

s
r
c 1

t
i
t
l
e
= "Cf-252 neutrons, Watt fission spectrum model"
```

(continues on next page)

(continued from previous page)

```
s
t
r
e
n
g
t
h=4.05E+07

c
u
b
o
i
d  0
.01 0
.01  0 0  0 0

n
e
u
t
r
o
n
s

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources

'------------------------------------------------------------------------------
' Tallies Block
'------------------------------------------------------------------------------
read
 tallies

p
o
i
n
t
D
e
t
e
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="center of detector"

l
o
c
a
t
i
o
n
I
D
=1

r
e
s
p
o
n
s
e
I
D
=5
    end
 pointDetector

m
e
s
h
T
a
l
l
y 1

t
i
t
l
e
="example mesh tally"

g
r
i
d
G
e
o
m
e
t
r
y
I
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e
I
D
=5

n
o
G
r
o
u
p
F
l
u
x
e
s
    end
 meshTally
end
 tallies

'------------------------------------------------------------------------------
' Parameters Block
'------------------------------------------------------------------------------
read
 parameters

r
a
n
d
o
m
S
e
e
d
=00003
e
c
d7
b4
e3
e8
b

l
i
b
r
a
r
y
="v7-200n47g"
```

(continues on next page)

(continued from previous page)

```
p
e
r
B
a
t
c
h
=10000
b
a
t
c
h
e
s
=10

f
i
s
s
i
o
n
M
u
l
t
=0
n
o
P
h
o
t
o
n
s
end
 parameters

'-----------------------------------------------------------------------------
' Importance Map Block
'-----------------------------------------------------------------------------
read
 importanceMap

a
d
j
o
i
n
t
S
o
u
r
c
e 1
```

(continues on next page)

(continued from previous page)

```
l
o
c
a
t
i
o
n
I
D
=1

r
e
s
p
o
n
s
e
I
D
=5
    end
 adjointSource

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=7

m
a
c
r
o
m
a
t
e
r
i
a
l

m
m
T
o
l
e
r
```

(continues on next page)

(continued from previous page)

```
    end
 macromaterial
end
 importanceMap

end
 data
end
```

Output

MAVRIC results for the point detector response for the 20 cm case are shown below and in Fig. 1.5.

```
N
e
u
t
r
o
n
P
o
i
n
t
D
e
t
e
c
t
o
r 1
.
c
e
n
t
e
r
o
f
d
e
t
e
c
t
o
r

a
v
e
r
a
g
e
s
t
a
n
```

(continues on next page)

(continued from previous page)

```
t
a
l
l
y
/
q
u
a
n
t
i
t
y
v
a
l
u
e
d
e
v
i
a
t
i
o
n
u
n
c
e
r
t
(
/
m
i
n
)   1 2 3 4 5 6

-
-
-
```

(continued from previous page)

```
u
n
c
o
l
l
i
d
e
d
f
l
u
x     1
.06384
E
+01  1
.88744
E
-02  0
.00177

t
o
t
a
l
f
l
u
x          2
.36367
E
+02  5
.47276
E
+00  0
.02315  8
.10
E
+02
X
-
X
-
X
-

r
e
s
p
o
n
s
e 5          1
.28632
E
-02  1
.74351
E
-04  0
.01355  2
```

(continues on next page)

(continued from previous page)

(continues on next page)

(continued from previous page)

This problem took only ~2.5 minutes (0.2 in Denovo and 2.3 minutes in Monaco) on the same processor as the 20 minute analog case. (The figure of merit [FOM] is 15 times higher than the analog.) Note that the point detector dose rate is the same as the Monaco analog sample problem, but the relative uncertainty is smaller with less computation time. CADIS has optimized the calculation by focusing on neutrons that contribute to the dose rate at the detector location at the expense of neutrons in the paraffin block. This is demonstrated by the mesh tally of dose rates where the values for the dose rate are lower in the paraffin block and the relative uncertainties are higher. Since the calculation was optimized for the position of the detector, dose rates in other parts of the problem are underestimated and should not be believed.

The mesh tally shows that the CADIS calculation did not follow as many particles deep into the paraffin block, so the uncertainties are greater there, but that is what this problem was supposed to do—reduce the uncertainty at the point detector at the expense of the other portions of the problem.

Fig. 1.5: Mesh tally showing neutron dose rate (rem/hr) and uncertainties for the analog case and the CADIS case.

1.5.2 Dose rates outside of a simple cask

This example problem is a full-size cylindrical cask model, which consists of an inner steel liner, a thick section of concrete, and an outer steel cover. This problem is intended to be used as a tool to teach users how to build MAVRIC input files. This is not a completely realistic shipping cask; it has been simplified greatly for this purpose. The goal of this example it to show how to quickly calculate neutron and photon does rates at six points outside of the cask, including in front of the vent port.

Geometry and materials

The simple model of a cask is shown in Fig. 1.6. Vent ports at the top and bottom of the cask are modeled as void all of the way around the cask. The interior of the cask was modeled using materials from about 20 typical pressurized water reactor (PWR) fuel assemblies (including the UO2, Zr, Fe, Ni, Cr, Sn, and other constituents), homogenized over the interior volume. The total mass of the fuel/assembly hardware in this region is 10.6 metric tonnes. Separate end regions of the assemblies are not modeled in this simple example. Also note that the fuel material is based on fresh fuel, not spent fuel with its hundreds of fission products.

Model Specifics

Materials
fuel: UO_2, Zr, others, ρ=0.9137 g/cm^3
stainless steel :SCALE ss304, ρ=7.94 g/cm^3
concrete :SCALE orconcrete, ρ=2.2994 g/cm^3

Regions (r_{min}, r_{max}, z_{min}, z_{max}, all in cm)
yellow: 0, 95, -228.6, 228.6; fuel
blue: 95, 100, -255.2 255.2; inner steel liner
blue: 0, 90, 228.6, 240.6; inner steel liner
blue: 0, 90, -240.6, -228.6; inner steel liner
gray: 100,168, -255.2, 255.2; concrete
gray: 0, 90, 240.6, 280.6; concrete
gray: 0, 90, -280.6, -240.6; concrete
blue: 168, 170, -255.2 255.2; outer steel liner
blue: 0, 170, 280.6.2, 285.6; outer steel liner
blue: 0, 170, -285.6, -280.6.2; outer steel liner

Detector locations (coordinates in cm)
1: 180, 0, 0; midplane, 10 cm from surface
2: 0, 0, 295.6; on axis, 10 cm from surface
3: 180, 0, 267.9; center of gap, 10 cm from r_{max}
4: 270, 0, 0; midplane, 100 cm from surface
5: 0, 0, 385.6; on axis, 100 cm from surface
6: 270, 0, 385.6; 100 cm from each surface

Fig. 1.6: Cask geometry and detector locations.

Sources and responses

Spent fuel from a typical mid-sized PWR was used to determine the source term. ORIGEN was used to deplete a full core (46.1 metric tonnes of uranium, 4.2% enriched, with O, Zr, Fe, Ni, Cr, Sn, and other constituents) to 55,000 MWdays/MTU. The contents of the modeled fuel represent typical values for PWR fuel. ORIGEN then computed the neutron and photon spectra in 27-group and 19-group energy structures for the fuel following a 10-year cooling period after the last irradiation. The total neutron source strength for the cask (1/6 of a full core, or about 20 assemblies) was 8.577×10^9 neutrons/s. The total photon source strength was 7.155×10^{16} photons/s.

Two cases will be done for this example: one for calculating the neutron dose rates from the spent fuel neutrons and the other for calculating the photon dose rates from the spent fuel photons. The source spectra and response functions are shown in Fig. 1.7 through Fig. 1.10 and listed in Table 1.9. Note that in this example, the neutron source shown in Fig. 1.7 and Table 1.9 is considered the final neutron source: no further neutron multiplication is considered.

Fig. 1.7: Spent fuel neutron source spectrum with strength 8.577×10^9/second.

Table 1.9: Source and response data using the SCALE 27-group energy structure for neutrons and the 19-group energy structure for photons

	Energy	neutron	response		Energy	photon	response
	(eV)	source	9029		(eV)	source	9504
	2.0000E+07	2.040E-02	1.615E-04		2.00E+07	1.320E-12	1.162E-05
	6.3763E+06	2.147E-01	1.445E-04		1.00E+07	7.185E-11	8.745E-06
	3.0119E+06	2.365E-01	1.270E-04		8.00E+06	3.281E-10	7.460E-06
	1.8268E+06	1.267E-01	1.281E-04		6.50E+06	1.672E-09	6.351E-06
	1.4227E+06	1.586E-01	1.298E-04		5.00E+06	4.167E-09	5.400E-06

continues on next page

Table 1.9 – continued from previous page

	9.0718E+05	1.587E-01	1.034E-04		4.00E+06	8.086E-08	4.602E-06
	4.0762E+05	7.281E-02	5.266E-05		3.00E+06	7.937E-07	3.952E-06
	1.1109E+05	1.073E-02	1.286E-05		2.50E+06	1.164E-05	3.459E-06
	1.5034E+04	7.688E-04	3.736E-06		2.00E+06	3.331E-05	3.013E-06
	3.0354E+03	5.694E-05	3.720E-06		1.66E+06	8.160E-03	2.620E-06
	5.8295E+02	4.479E-06	4.009E-06		1.33E+06	3.511E-02	2.194E-06
	1.0130E+02	3.148E-07	4.295E-06		1.00E+06	2.478E-02	1.827E-06
	2.9023E+01	4.983E-08	4.473E-06		8.00E+05	4.827E-01	1.515E-06
	1.0677E+01	9.864E-09	4.566E-06		6.00E+05	4.641E-02	1.160E-06
	3.0590E+00	1.117E-09	4.560E-06		4.00E+05	9.735E-03	8.705E-07
	1.8554E+00	3.286E-10	4.521E-06		3.00E+05	1.514E-02	6.219E-07
	1.3000E+00	1.060E-10	4.487E-06		2.00E+05	5.182E-02	3.708E-07
	1.1253E+00	9.203E-11	4.466E-06		1.00E+05	7.015E-02	2.688E-07
	1.0000E+00	9.135E-11	4.434E-06		4.50E+04	2.560E-01	5.933E-07
	8.0000E-01	1.755E-10	4.332E-06		1.00E+04		
	4.1399E-01	2.590E-11	4.203E-06				
	3.2500E-01	3.024E-11	4.097E-06				
	2.2500E-01	3.451E-11	3.840E-06				
	1.0000E-01	3.269E-12	3.675E-06				
	5.0000E-02	5.447E-12	3.675E-06				
	3.0000E-02	4.089E-14	3.675E-06				
	1.0000E-02	4.916E-14	3.675E-06				
	1.0000E-05						

Energies listed are the bin upper energies. Source units are particles/s normalized to a total of 1 particle/s. Response units are (rem/hr)/(particle/cm^2/s).

Analog calculation

The analog model for this problem starts with the problem title and the cross section library name, which in this example is the ENDF/B-VII.0 27 neutron group / 19 photon group library. This is in the SCALE `samples\input` directory as `mavric.caskAnalogn.inp` and `mavric.caskAnalogp.inp`.

```
=mavric

S
i
m
p
l
i
f
i
e
d
c
a
s
k
m
o
d
```

(continues on next page)

Fig. 1.8: ANSI-1977/ flux-to-dose-rate factors (rem/hr)/(neutrons/cm ^{2}/sec).

Fig. 1.9: Spent fuel photon source spectrum with strength 7.155×10^{16}/second

Fig. 1.10: ANSI-1977 photon flux-to-dose-rate factors (rem/hr)/(photons/cm ^{2}/sec)

(continued from previous page)

```
v7
-27
n19
g
```

Then the material compositions are listed for fresh fuel, concrete, and steel.

```
read
 composition

w
t
p
t
F
u
e
l   1 0
.913717475 18         6000  0
.00939719    7014  0
.00528993
                    8016  9
.73397641   13000  0
.00715715   14000  0
.01031670
                   15000  0
.02227505   22000  0
.00780567   24000  0
.36655141
                   25000  0
.01716839   26000  0
.72041451   27000  0
.00523824
                   28000  0
.68955526   40000 15
.78990702   41000  0
.05130153
                   42000  0
.02844690   50118  0
.25877903   92235  3
.03560962
                   92238 69
.24080999
                 1
.0 293
.0 end

o
r
c
o
n
c
r
e
t
e 2 1
.0 293
.0 end
```

(continues on next page)

(continued from previous page)

```
s
s304       3 1
.0 293
.0 end
end
 composition
```

Then the SGGP geometry is listed, with the origin of the coordinate system at the center of the cask.

```
read
 geometry

g
l
o
b
a
l
u
n
i
t  1

z
c
y
l
i
n
d
e
r  1   95
.0  228
.6
-228
.6

z
c
y
l
i
n
d
e
r  2  170
.0  255
.2
-255
.2

z
c
y
l
i
```

(continues on next page)

```
n
d
e
r  3   90
.0  240
.6
-240
```

(continued from previous page)

```
z
c
y
l
i
n
d
e
r  4   90
.0  280
.6
-280
.6

z
c
y
l
i
n
d
e
r  5  170
.0  280
.6
-280
.6

z
c
y
l
i
n
d
e
r  6  170
.0  285
.6
-285
.6

z
c
y
l
i
n
d
e
r  7   95
.0  255
.2
-255
.2
```

(continues on next page)

```
z
c
y
l
i
n
d
```

(continued from previous page)

```
z
c
y
l
i
n
d
e
r  9  168
.0  255
.2
-255
.2

s
p
h
e
r
e    10  999
.0

m
e
d
i
a  1 1   1
v
o
l=1.29629E+07

m
e
d
i
a  3 1   8
-7
v
o
l=1.56338E+06

m
e
d
i
a  2 1   9
-8
v
o
l=2.92216E+07

m
e
d
i
a  3 1   2
-9
v
o
l=1.08594E+06
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  3 1   3
-1
v
o
l=6.10726E+05

m
e
d
i
a  2 1   4
-3
v
o
l=2.03575E+06

m
e
d
i
a  3 1   6
-5
v
o
l=9.07920E+05

m
e
d
i
a  0 1   5
-4
-2
v
o
l=3.31953E+06

m
e
d
i
a  0 1   7
-4
-1
v
o
l=1.54598E+05

m
e
d
i
a  0 1   10
-6
v
o
l=4.12429E+09
```

(continues on next page)

(continued from previous page)

```
b
o
u
n
d
a
r
y 10
end
 geometry
```

The definitions block contains locations, response functions, grid geometries, and a distribution used by the source input block. For the neutron source/neutron dose problem, the definitions block is listed below.

```
read
 definitions

l
o
c
a
t
i
o
n 1
p
o
s
i
t
i
o
n 180
.0 0
.0   0
.0    end
 location

l
o
c
a
t
i
o
n 2
p
o
s
i
t
i
o
n   0
.0 0
.0 295
.6    end
 location
```

(continues on next page)

(continued from previous page)

```
l
o
c
a
t
i
o
n 3
p
o
s
i
t
i
o
n 180
.0 0
.0 267
.9    end
 location

l
o
c
a
t
i
o
n 4
p
o
s
i
t
i
o
n 270
.0 0
.0   0
.0    end
 location

l
o
c
a
t
i
o
n 5
p
o
s
i
t
i
```

(continues on next page)

```
o
n   0
.0 0
.0 385
.6    end
 location
```

(continued from previous page)

```
l
o
c
a
t
i
o
n 6
p
o
s
i
t
i
o
n 270
.0 0
.0 385
.6    end
 location

r
e
s
p
o
n
s
e 1
s
p
e
c
i
a
l
D
o
s
e
=9029  end
 response

d
i
s
t
r
i
b
u
t
i
o
n 1
```

(continues on next page)

```
t
i
t
l
e
="kewaunee core, 3 cycles and then 10 years"
```

(continued from previous page)

```
n
e
u
t
r
o
n
G
r
o
u
p
s

t
r
u
e
P
D
F  2
.040
E
-02 2
.147
E
-01 2
.365
E
-01 1
.267
E
-01 1.586E-01
                 1
.587
E
-01 7
.281
E
-02 1
.073
E
-02 7
.688
E
-04 5.694E-05
                 4
.479
E
-06 3
.148
E
-07 4
.983
E
-08 9
```

(continues on next page)

```
.864
E
-09 1.117E-09
```

(continued from previous page)

```
                    3
.286
E
-10 1
.060
E
-10 9
.203
E
-11 9
.135
E
-11 1.755E-10
                    2
.590
E
-11 3
.024
E
-11 3
.451
E
-11 3
.269
E
-12 5.447E-12
                    4
.089
E
-14 4
.916
E
-14 end
    end
 distribution
end
 definitions
```

The neutron source from the spent fuel is then listed.

```
read
 sources

s
r
c 1

t
i
t
l
e
="1/6 of kewaunee core, ~ 0.25 Ci"

s
t
r
e
n
g
t
h=8.577E+09
```

(continues on next page)

(continued from previous page)

```
n
e
u
t
r
o
n
s

z
C
y
l
i
n
d
e
r 95
.0  228
.6
-228
.6

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources
```

Six point detectors are used to evaluate dose rates radially, axially, and near the vent port.

```
read
 tallies

p
o
i
n
t
D
e
t
e
c
t
o
r 1
l
```

(continues on next page)

(continued from previous page)

```
p
o
i
n
t
D
e
t
e
c
t
o
r 2
l
o
c
a
t
i
o
n
I
D
=2
r
e
s
p
o
n
s
e
I
D
=1  end
 pointDetector

p
o
i
n
t
D
e
t
e
c
t
o
r 3
l
o
c
a
t
i
o
n
I
D
=3
r
e
```

(continues on next page)

(continued from previous page)

```
p
o
i
n
t
D
e
t
e
c
t
o
r 4
l
o
c
a
t
i
o
n
I
D
=4
r
e
s
p
o
n
s
e
I
D
=1  end
 pointDetector

p
o
i
n
t
D
e
t
e
c
t
o
r 5
l
o
c
a
t
i
o
n
I
D
=5
r
e
```

(continues on next page)

(continued from previous page)

```
p
o
i
n
t
D
e
t
e
c
t
o
r 6
l
o
c
a
t
i
o
n
I
D
=6
r
e
s
p
o
n
s
e
I
D
=1  end
 pointDetector
end
 tallies
```

The Monte Carlo parameters were tailored for the neutron problem to be 1-minute batches on a 2 GHz Linux computer. For the photon problem, the number per batch would be 91,000 for 1-minute batches.

```
read
 parameters

r
a
n
d
o
m
S
e
e
d
=8655745280030001
```

(continues on next page)

(continued from previous page)

```
p
e
r
B
a
t
c
h
=25400
b
a
t
c
h
e
s
=600

f
i
s
s
i
o
n
M
u
l
t
=0
n
o
P
h
o
t
o
n
s
end
 parameters
```

No biasing is specified, which will use the default weight window target value of 1 for every energy group in every region. To allow the neutrons to penetrate into the cask wall before being rouletted, a larger window ratio is used, making the lower weight window bound 0.01.

```
read
 biasing

w
i
n
d
o
w
R
```

(continues on next page)

```
a
t
i
o
=199
.0
```

(continued from previous page)

```
end
 biasing
```

The Monaco input is then ended.

```
end
 data
end
```

For the photon source/photon dose rate problem, the definitions block would instead contain a photon flux-to-dose-rate response function and the energy distribution for the source.

```
read
 definitions

r
e
s
p
o
n
s
e 1

s
p
e
c
i
a
l
D
o
s
e
=9504
    end
 response

...

d
i
s
t
r
i
b
u
t
i
o
n 1

t
i
t
l
e
="kewaunee core, 3 cycles and then 10 years"
```

(continues on next page)

(continued from previous page)

```
p
h
o
t
o
n
G
r
o
u
p
s

t
r
u
e
P
D
F 1
.320
E
-12 7
.185
E
-11 3
.281
E
-10 1
.672
E
-09 4.167E-09
                8
.086
E
-08 7
.937
E
-07 1
.164
E
-05 3
.331
E
-05 8.160E-03
                3
.511
E
-02 2
.478
E
-02 4
.827
E
-01 4
.641
E
-02 9.736E-03
```

(continues on next page)

(continued from previous page)

```
                1
.514
E
-02 5
.182
E
-02 7
.015
E
-02 2
.560
E
-01       end
    end
 distribution
end
 definitions
```

The sources block would contain the photon source information.

```
read
 sources

s
r
c 1

t
i
t
l
e
="1/6 of kewaunee core, ~ 2e6 Ci"

s
t
r
e
n
g
t
h=7.155e+16

p
h
o
t
o
n
s

z
C
y
l
i
n
d
e
r 95
.0  228
.6
-228
.6
```

(continues on next page)

(continued from previous page)

```
e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources
```

Each of the two analog problems in the `samples\input` directory will run for about 10 minutes. In this time, no meaningful results will be generated due to the difficulty of the problem. Analog results for each case running 110 hr are listed in Table 1.10 for the neutron source/neutron dose problem, while results for the photon problem are listed in Table 1.11. Note that after 110 hr, some of the relative uncertainties in the point detector tallies are still quite high, and only one of the six tallies in each problem passed all of the statistical checks. Fig. 1.11 is the convergence plot for the neutron dose rate at point detector 1, showing that the tally is not well converged and that some batches contain rare events that change the tally value a great deal.

Table 1.10: Analog Monaco results for the simplified cask model—neutron source/neutron dose rate.

	Dose Rate	relative
detector	(rem/hr)	uncertainty
1	8.78E-04	0.1853
2	7.35E-03	0.0408
3	1.54E-02	0.0124
4	4.47E-04	0.0311
5	1.36E-02	0.0058
6	2.92E-03	0.0073

Table 1.11: Analog Monaco results for the simplified cask model—photon source/photon dose rate.

	Dose Rate	relative
detector	(rem/hr)	uncertainty
1	2.66E-02	0.2713
2	3.05E-01	0.0787
3	2.97E+00	0.0199
4	2.65E-02	0.1345
5	3.26E+00	0.0133
6	3.30E-01	0.0244

Fig. 1.11: Convergence plot for the neutron dose rate at point detector 1 (error bars show the 1-sigma tally uncertainties).

SAS4 calculations

Calculations for these two problems were also done using the SAS4 sequence in SCALE 5.1. SAS4 was specifically designed for cask geometries and used a one-dimensional discrete-ordinates calculation (either radially or axially) to determine weight windows. Results for the neutron problem are shown in Table 1.12, and results for the photon problem are shown in Table 1.13. Note that SAS4 using radial biasing is only expected to do well for the two radial point detector locations. Similarly, only the two axial point detectors are expected to do well when using axial biasing. SAS4 was not intended to do well for the points near the vent port, but the results using the axial biasing seem reasonable.

Table 1.12: SAS4 results using radial biasing (361 minutes) and axial biasing (361 minutes), for the simplified cask model—neutron source/neutron dose rate

	Radial Biasing		Axial Biasing	
	Dose Rate	relative	Dose Rate	relative
detector	(rem/hr)	uncertainty	(rem/hr)	uncertainty
1	7.67E-04	0.0081	1.32E-05	0.4453
2	2.67E-02	0.8623	7.80E-03	0.0040
3	1.27E-02	0.1425	1.53E-02	0.0079
4	4.54E-04	0.0079	2.34E-04	0.6780
5	1.43E-02	0.1349	1.35E-02	0.0044
6	2.81E-03	0.1274	2.86E-03	0.0052

Table 1.13: SAS4 results using radial biasing (361 minutes) and axial biasing (361 minutes), for the simplified cask model—photon source/photon dose rate

	Radial Biasing		Axial Biasing	
	Dose Rate	relative	Dose Rate	relative
detector	(rem/hr)	uncertainty	(rem/hr)	uncertainty
1	4.54E-02	0.0118	7.07E-04	0.5375
2	6.74E-02	0.3295	2.45E-01	0.0630
3	5.63E-01	0.3818	2.07E+00	0.2289
4	2.76E-02	0.0039	2.48E-03	0.4570
5	1.85E+00	0.1699	2.70E+00	0.0664
6	1.46E-01	0.1493	2.73E-01	0.0838

Calculations using CADIS

In the analog calculations, the dose rates at all six points could be calculated at the same time. With MAVRIC and using CADIS, the importance map will optimize the transport of particles towards only the selected detector. Hence, each detector will have a separate calculation with an importance map tailored to reduce the variance for only that detector. Calculations for close detectors could be performed at the same time. For example, detectors 1 and 4 both need to push particles out of the cask in the positive x direction, towards the z=0 plane. In this example, all six detectors will use separate importance maps.

For the importance map, in the input, the user lists what planes to use for the adjoint discrete-ordinates calculation. These planes define cells, which are treated as homogenous parallelpipeds by Denovo, made of a macro material corresponding to a mixture of materials that are in the cell in the true geometry. Users should try to bound as many materials as possible with their selection of mesh planes. More mesh planes should be used where the importance (adjoint flux) varies quickly, such as near the adjoint sources (the detector positions). It is also important to have planes on the true source bounding box.

In this example problem, different sets of mesh planes will be used for the different detector positions. For detector positions 1 and 4, the mesh planes are shown in Fig. 1.12 and Fig. 1.13. Note that there are more planes closer to the detectors. Also note that in the z dimension, it is quite easy to place mesh planes at every material boundary, but it is a bit more difficult to do so in the x and y dimensions due to the curved surfaces. Users need not worry about getting things perfect—an approximate importance map can still reduce Monte Carlo variances a great deal. The meshes used

for detector positions 2/5 and positions 3/6 are also shown in Fig. 1.12 and Fig. 1.13. Mesh parameters are listed in Table 1.14, and the mesh planes are listed in Table 1.15.

Fig. 1.12: Importance map mesh planes in the x and z dimensions for detector positions 1/4, 2/5, and 3/6.

Fig. 1.13: Importance map mesh planes in the x and y dimensions for detector positions 1/4, 2/5, and 3/6.

Table 1.14: Mesh parameters

Detector position	Number	of	cells	Total cells
	x	y	z	
1/4	46	35	35	56350
2/5	35	35	49	60025
3/6	46	35	49	78890

Table 1.15: List of the various sets of mesh planes used for the importance calculations for six different point detectors

x		x		y		z		z	
1,3,4,6		2,5		1,2,3,4,5,6		1,4		2,3,5,6	
-170	108	-170	5	-170	5	-285.6	3	-285.6	190
-168	112	-168	15	-168	15	-280.6	10	-280.6	210
-146	116	-155	25	-155	25	-255.2	20	-255.2	216.2
-122	120	-141	35	-141	35	-240.6	30	-240.6	222.4
-100	124	-127	45	-127	45	-228.6	40	-228.6	228.6
-95	128	-113	55	-113	55	-200	50	-210	232.6
-90	132	-100	65	-100	65	-160	60	-190	236.6
-60	136	-95	75	-95	75	-120	70	-170	240.6
-40	140	-90	85	-90	85	-100	80	-150	245.1
-20	144	-85	90	-85	90	-80	100	-130	249.7
-5	148	-75	95	-75	95	-70	120	-110	254.2
5	152	-65	100	-65	100	-60	160	-90	255.2
15	156	-55	113	-55	113	-50	200	-70	256.2
25	158	-45	127	-45	127	-40	228.6	-50	260.1
35	160	-35	141	-35	141	-30	240.6	-30	264
45	162	-25	155	-25	155	-20	255.2	-10	267.9
55	164	-15	168	-15	168	-10	280.6	10	271.8
65	165	-5	170	-5	170	-3	285.6	30	275.7
75	166							50	279.6
85	167							70	280.6
90	168							90	281.6
95	169							110	282.6
100	170							130	283.6
104								150	284.6
								170	285.6

MAVRIC input files

With two sources and six detectors, this example problem will require 12 separate input files. Starting with the two input files for the analog calculations, these 12 input files will share most of the same features and will differ only in blocks related to the importance map calculation: the location of the adjoint source and the planes used in the grid geometry.

To change the input for the neutron problem from an analog calculation to one using CADIS, the user first adds the mesh planes for the discrete-ordinates calculation as a grid geometry to the definitions block. This set of planes is tailored for the vent port direction toward detectors 3 and 6.

```
gridGeometry 3
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="for importance map for detectors 3,6"

x
p
l
a
n
e
s
-170
-168
-146
-122
-100

-95
-90
-60
-40
-20
-5
                5 15 25 35 45 55 65 75 85 90 95 100
                104 108 112 116 120 124 128 132 136 140 144 148 152
                156 158 160 162
                164 165 166 167
                168 169 170  end

y
p
l
a
n
e
s
-170
-168
-155
-141
-127
-113
-100

-95
-90
-85
-75
-65
-55
-45
-35
-25
-15
-5
```

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(continued from previous page)

```
                5 15 25 35 45 55 65 75 85 90 95 100
                113 127 141 155 168 170  end

z
p
l
a
n
e
s
-285
.6
-280
.6
-255
.2
-240
.6
-228
.6
-210

-190
-170
-150
-130
-110
-90
-70
-50
-30
-10
                10 30 50 70 90 110 130 150 170 190
                210    216
.2 222
.4
                228
.6  232
.6 236
.6
                240
.6  245
.1 249
.7 254
.2
                255
.2  256
.2 260
.1 264 267
.9 271
.8 275
.7 279
.6
                280
.6  281
.6 282
.6 283
.6 284
.6 285
.6  end
```

(continues on next page)

(continued from previous page)

```
end
 gridGeometry
```

To help the mesh-based biased source represent the true source, "mixture=1" can be added to the source definition. This will ensure that particles sampled from the mesh source that are not in the fuel are rejected. Then an importance map block replaces the standard biasing block. In this case, the importance map will optimize the flow of particles to location 3 (where point detector 3 is defined).

```
read
 importanceMap

a
d
j
o
i
n
t
S
o
u
r
c
e 1

l
o
c
a
t
i
o
n
I
D
=3

r
e
s
p
o
n
s
e
I
D
=1
    end
 adjointSource

g
r
i
d
G
e
o
m
e
t
r
y
I
```

(continues on next page)

(continued from previous page)

```
m
a
c
r
o
m
a
t
e
r
i
a
l

m
m
T
o
l
e
r
a
n
c
e
=0
.01
    end
 macromaterial
end
 importanceMap
```

A mesh tally could be added with the following in the tallies block.

```
meshTally 1
      title="Shows how importance map changes the transport of particles"
      gridGeometryID=3
      responseID=1
end meshTally
```

The above mesh tally uses the same grid geometry as the CADIS calculations, but a different grid (or grids) could be used. The files `mavric.caskCADISn.inp` and `mavric.caskCADISp.inp` are available in the SCALE `samples\input` directory. These are for calculating the dose rates at detector position 3, but they can be modified for the other five positions (by changing the geometry grid planes and the adjoint source location).

Neutron source/neutron response results

The above MAVRIC input file first performed the discrete-ordinates calculation to determine the adjoint flux from detector position 3. The adjoint Denovo flux file (*.adjoint.dff) produced can be viewed using the Mesh File Viewer and is shown in Fig. 1.14 for several of the neutron energy groups.

MAVRIC then combined a mesh representation of the true source (space and energy) with the adjoint fluxes to create the importance map and mesh-based biased source. These are shown in Fig. 1.15 for the fifth neutron group, covering the energy range of 0.9 to 1.4 MeV. Notice how the most important region (lowest target weights) is right around the vent port near detector position 3. This is something we know qualitatively, but quantitative values for exactly how the importance changes with space and energy are difficult to guess. Also notice the "consistent" part of CADIS——the source particles—are born with a weight that matches the target weight for the position they are born into. The biased source sampling distribution is depicted in Fig. 1.16, showing how the source particles nearest to detector 3 will be sampled more often.

The biased source distribution and the importance map are then used by Monaco to compute the dose equivalent rate response at detector 3.

The results for all six neutron cases, each using their own importance map and biased source, are shown in Table 1.16.

This example shows that MAVRIC using CADIS obtains the correct answer much faster than the analog calculations. This is shown with a comparison to the results from the analog Monaco and SAS4 calculations, all of which are listed in Table 1.17.

To account for the time it takes to achieve a given level of uncertainties, the calculation figure-of-merit—FOM=1/time/(relative uncertainty)^2—can be calculated for each of the codes. The ratios of each code FOM to the FOM of analog Monaco (speedup) are listed in Table 1.18 to show how much faster MAVRIC and SAS4 are compared to analog Monaco. The FOMs for MAVRIC include the Denovo calculation times. The FOMs for analog Monaco and SAS4 were modified to account for calculating all six detectors at once.

Fig. 1.14: Adjoint neutron fluxes (/cm ^{2}/s) for groups 5 (0.9–1.4 MeV), 10 (0.58–3.0 keV), and 19 (0.8–1 eV) calculated by Denovo.

Fig. 1.15: Neutron target weights from the importance map and source weights (at birth) for neutron group 5 (0.9 to 1.4 MeV).

Fig. 1.16: Biased source sampling probability (neutrons/cm3) for neutron groups 5 (0.9-1.4 MeV), 10 (0.58–3.0 keV), and 19 (0.8–1 eV).

Table 1.16: Final MAVRIC results (rem/hr) for each point detector in the neutron source/neutron dose rate problem

	Time (minutes)		Dose Rate	relative
detector	Denovo	Monaco	(rem/hr)	uncertainty
1	6.9	131	7.65E-04	0.0081
2	7.8	64	7.83E-03	0.0030
3	9.8	65	1.54E-02	0.0029
4	6.4	120	4.57E-04	0.0029
5	7.3	64	1.36E-02	0.0028
6	9.5	65	2.93E-03	0.0023

Table 1.17: Comparison of neutron dose rates (rem/hr) to other SCALE codes

	Analog Monaco	SAS4 radial	SAS4 axial	MAVRIC
detector	6595 min	360 min	361 min	556 min
1	8.78E-04 ± 19%	7.67E-04 ± 0.8%	1.32E-05 ± 45%	7.65E-04 ± 0.8%
2	7.35E-03 ± 4.1%	2.67E-02 ± 86%	7.80E-03 ± 0.4%	7.83E-03 ± 0.3%
3	1.54E-02 ± 1.2%	1.27E-02 ± 14%	1.53E-02 ± 0.8%	1.54E-02 ± 0.3%
4	4.47E-04 ± 3.1%	4.54E-04 ± 0.8%	2.34E-04 ± 68%	4.57E-04 ± 0.3%
5	1.36E-02 ± 0.6%	1.43E-02 ± 13%	1.35E-02 ± 0.4%	1.36E-02 ± 0.3%
6	2.92E-03 ± 0.7%	2.81E-03 ± 12.7%	2.86E-03 ± 0.5%	2.93E-03 ± 0.2%

Table 1.18: Ratio of the figure-of-merit (speed-up) of MAVRIC and SAS4 compared to analog Monaco :header-rows:m

			SAS4	SAS4		
	detector	Monaco	radial	axial	MAVRIC	
	1	1	9498	3.2	4178	
	2	1	0.0	1874	2858	
	3	1	0.1	45	270	
	4	1	287	0.0	1002	
	5	1	0.0	32	65	
	6	1	0.1	35.8	146	

Photon source/photon response results

The results for the photon source/photon response are similar to the results of the neutron source/neutron response. For the MAVRIC calculation using the photon importance map made from an adjoint source located at detector position 3, Fig. 1.17 details the adjoint photon flux. Fig. 1.18 compares the target weights from the importance map and the source birth weights. Fig. 1.19 shows the distribution of the sampled source positions from the biased source.

Table 1.19 shows the results from all six photon MAVRIC runs, each using its own importance map and biased source.

The MAVRIC results of the photon problem compare well against SAS4 and analog Monaco, as shown in Table 1.20 and Table 1.21.

Fig. 1.17: Adjoint photon fluxes (/cm: sup:2/s) for groups 2 (8–10 MeV), 2 (0.8–1.0 MeV), and 18 (45–100 keV) calculated by Denovo.

Table 1.19: Final MAVRIC results (rem/hr) for each point detectorin the photon source/photon dose rate problem

	Time (minutes)		Dose Rate	relative
detector	Denovo	Monaco	(rem/hr)	uncertainty
1	2.6	121	5.02E-02	0.0024
2	3.1	65	3.03E-01	0.0177
3	3.6	64	2.89E+00	0.0105
4	2.6	130	3.18E-02	0.0024
5	3.1	59	3.07E+00	0.0156
6	3.8	63	3.14E-01	0.0137

Fig. 1.18: Photon target weights from the importance map and source weights (at birth) for photon group 12 (0.8–1.0 MeV).

Table 1.20: Comparison of the photon dose rates (rem/hr) to other SCALE codes

		Analog Monaco		SAS4 radial		SAS4 axial		MAVRIC		
	detector	6678 min		361 min		361 min		520 min		
	1	2.66E-02	± 27%	4.54E-02	± 1.2%	7.07E-04	± 54%	5.02E-02	± 0.2%	
	2	3.05E-01	± 7.9%	6.74E-02	± 33%	2.45E-01	± 6.3%	3.03E-01	± 1.8%	
	3	2.97E+00	± 2.0%	5.63E-01	± 38%	2.07E+00	± 22.9%	2.89E+00	± 1.0%	
	4	2.65E-02	± 13.4%	2.76E-02	± 0.4%	2.48E-03	± 46%	3.18E-02	± 0.2%	
	5	3.26E+00	± 1.3%	1.85E+00	± 17%	2.70E+00	± 6.6%	3.07E+00	± 1.6%	
	6	3.30E-01	± 2.4%	1.46E-01	± 14.9%	2.73E-01	± 8.4%	3.14E-01	± 1.4%	

Fig. 1.19: Biased source sampling probability (photons/cm3) for groups 2 (8–10 MeV), 12 (0.8–1.0 MeV), and 18 (45–100 keV).

Table 1.21: Ratio of the FOM (speed-up) of MAVRIC and SAS4 compared to analog Monaco

			SAS4	SAS4	
detector	Monaco		radial	axial	MAVRIC
1	1		9759	4.7	114619
2	1		1.1	29	325
3	1		0.1	0	60
4	1		21570	1.6	26329
5	1		0.1	1	13
6	1		0.5	1.6	53

1.5.3 Gamma-ray litho-density logging tool using FW-CADIS

Consider a simple model of a gamma-ray litho-density tool [GV91][WH98] used in well-logging studies, shown in Fig. 1.20. This model uses a 10 cm diameter tool made of iron (with a tungsten density) in a 20 cm borehole filled with water. The near detector is a 2 cm diameter cylinder, 2 cm in length, located 20 cm from the source. The far detector is a 4 cm by 4 cm cylinder located 40 cm from the source. Each detector is made of NaI and collimated to look out into the formation. The source is contained in an angled collimator, aiming upward and into the formation. The collimators are filled with oxygen. The extent of the modeled formation is 100 × 100 × 140 cm. The source is an isotropic ^{137}Cs source emitting 10^{11} photons/s (661.7 keV). For these calculations, no response function is used—the goal of this example is to calculate the total photon flux within each detector volume.

Fig. 1.20: Cutaway view of the litho-density tool in a rock formation.

Fig. 1.21: Denovo mesh, y=0 plane.

Fig. 1.22: Denovo mesh, z=20 plane (through near detector).

Input file

The following input file represents the simple model of the litho-density tool. It lists of the file `mavric.lithoFW.inp` located in the SCALE `samples\input` directory. The 27 neutron group/19 photon group library based on ENDF/B-VII.0 data was used for the discrete-ordinates calculations, whereas the final Monte Carlo calculation used the 200 neutron group / 47 photon group library.

The input file starts with the problem title, the library for the importance calculations, and the materials.

```
=mavric

P
h
o
t
o
n
l
i
t
h
o
d
e
n
```

(continues on next page)

(continued from previous page)

```
v7
-27
n19
g

read
 composition

o           1
d
e
n
=1
.0                1
.0 293
.0 end

w
t
p
t
N
a
I     2 3
.67  2 11000 15
.337
                         53129 84
.663  1
.0 293
.0 end

i
r
o
n        3
d
e
n
=19
.3               1
.0 293
.0 end

h2
o         4                       1
.0 293
.0 end

w
t
p
t
C
a
C
O3   5 2
.36  4  1000  1
.0
```

(continues on next page)

(continued from previous page)

```
                              6000 11
.0
                              8016 51
.4
                             20000 36
.6    1
.0 293
.0 end
end
 composition
```

The geometry is relatively simple. Volumes are only needed for the regions where tallies will be made.

```
read
 geometry

g
l
o
b
a
l
u
n
i
t  1

z
c
y
l
i
n
d
e
r  2 1
.0 10
.0  0
.0
o
r
i
g
i
n
x
=5
.0
r
o
t
a
t
e
a1
=90
a2
=45
```

(continues on next page)

(continued from previous page)

```
z
c
y
l
i
n
d
e
r  3 1
.0 21
.0 19
.0
o
r
i
g
i
n
x
=5
.0

x
c
y
l
i
n
d
e
r  4 1
.0 10
.0  5
.0
o
r
i
g
i
n
z
=20
.0

z
c
y
l
i
n
d
e
r  5 2
.0 42
.0 38
.0
```

(continues on next page)

```
o
r
i
g
i
n
x
```

(continued from previous page)

```
x
c
y
l
i
n
d
e
r  6 2
.0 10
.0  5
.0
o
r
i
g
i
n
z
=40
.0


z
c
y
l
i
n
d
e
r  7  5
.0 100
-40
o
r
i
g
i
n
x
=5
.0

z
c
y
l
i
n
d
e
r 11 10
.0 100
-40
```

(continues on next page)

```
c
u
b
o
i
d    12 50
-50  50
```

(continued from previous page)

```
m
e
d
i
a   1 1   2 7

m
e
d
i
a   2 1   3
v
o
l
=6
.2831853072

m
e
d
i
a   1 1   4
-3 7

m
e
d
i
a   2 1   5
v
o
l
=50
.265482456

m
e
d
i
a   1 1   6
-5 7

m
e
d
i
a   3 1   7
-2
-3
-4
-5
-6

m
e
d
i
a   4 1   11
-7
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a   5 1   12
-11

b
o
u
n
d
a
r
y 12
end
 geometry
```

The definitions block lists the response (total photon flux) so that it can be understood by both libraries used in the problem. The mesh grid for the importance calculations used 49 × 43 × 59 = 124,313 mesh cells, with particular emphasis on geometric representation of the collimators to ensure accurate importance maps. This mesh grid is shown in Fig. 1.21 and Fig. 1.22. The source is represented by a distribution in which the most probable bin is located right near the 661.7 keV line, which can be translated into one photon group in either library (from 600 to 800 keV in the 27/19 library or from 600 to 700 keV in the 200/47 library).

```
read
 definitions

r
e
s
p
o
n
s
e 1

t
i
t
l
e
="for computing total photon flux"

p
h
o
t
o
n
B
o
u
n
d
s 1
.0
e4 2
.0
e7 end
```

(continues on next page)

(continued from previous page)

```
v
a
l
u
e
s          1
.0   1
.0 end
    end
 response

g
r
i
d
g
e
o
m
e
t
r
y 1

t
i
t
l
e
="entire formation"

x
p
l
a
n
e
s
-50
-40
-35
-30
-25
-20
-15

-10
-9
-8
-7
-6
-5
-4
-3
-2
-1
```

(continues on next page)

(continued from previous page)

```
                 0 1 2 3 3
.5 4 4
.5 5 5
.5 6 6
.5 7 8 9
                 10 11 12 13 14 15 16 17 18 19 20
                 22 24 26 28 30 35 40 50 end

y
p
l
a
n
e
s
-50
-40
-35
-30
-25
-20
-18
-16
-14
-12

-10
-9
-8
-7
-6
-5
-4
-3
-2
-1
.5
-1
-0
.5
                 0 0
.5 1 1
.5 2 3 4 5 6 7 8 9
                 10 12 14 16 18 20 25 35 40 50 end

z
p
l
a
n
e
s
-40
-30
-20
-15
-10
-5
```

(continues on next page)

(continued from previous page)

```
-4
-3
-2
-1 0 1 2 3 4 5 6 7 8 9 10
                12   14 16 17 18 18
.5
                19   19
.5 20 20
.5
                21   21
.5 22 23 24 26 28 30 32 34 36 37
                38   39 40 41
                42   43 44 46 48 50 55 60 65 70 80 90 100 end
    end
 gridgeometry

g
r
i
d
g
e
o
m
e
t
r
y 2

t
i
t
l
e
="y=0 plane in detail"

x
L
i
n
e
a
r 100
-50
.0  50
.0

y
L
i
n
e
a
r   1
-1
.0   1
.0
```

(continues on next page)

(continued from previous page)

```
z
L
i
n
e
a
r 140
-40
.0 100
.0
    end
 gridgeometry

d
i
s
t
r
i
b
u
t
i
o
n 1

t
i
t
l
e
="cesium-137 gammas/decay"

d
i
s
c
r
e
t
e 31817  32194  36304   36378   37255   283500    661657 end

t
r
u
e
p
d
f  0
.0199 0
.0364 0
.00348 0
.00672 0
.00213 0
.0000058 0
.851  end
```

(continues on next page)

(continued from previous page)

```
    end
 distribution
end
 definitions
```

The source is a simple point source. For more realistic calculations, the source strength could be modified so that the total energy emitted is preserved, $S' = S\left(\frac{661.7}{0.5}\left(700+600\right)\right)$, which uses the ratio of the line energy to the energy at the center of the group in the 200/47 library.

```
read
 sources

s
r
c 1

t
i
t
l
e
="Cs-137 Source: 661.7 keV"

s
t
r
e
n
g
t
h=1.0e11

p
h
o
t
o
n
s

s
p
h
e
r
e  0
.0
o
r
i
g
i
n
x
=5
.0
```

(continues on next page)

(continued from previous page)

```
e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources
```

Each detector is represented by a region tally. A mesh tally is made for one slice in *y* for visualization.

```
read
 tallies

r
e
g
i
o
n
T
a
l
l
y 1

p
h
o
t
o
n
u
n
i
t
=1
r
e
g
i
o
n
=2
```

(continues on next page)

(continued from previous page)

```
    end
 regionTally

r
e
g
i
o
n
T
a
l
l
y 2

p
h
o
t
o
n
u
n
i
t
=1
r
e
g
i
o
n
=4
    end
 regionTally

m
e
s
h
T
a
l
l
y 1

t
i
t
l
e
="mesh tally in just the y=0 plane"

p
h
o
t
```

(continues on next page)

```
o
n
```

(continued from previous page)

```
g
r
i
d
G
e
o
m
e
t
r
y
I
D
=2

n
o
G
r
o
u
p
F
l
u
x
e
s
    end
 meshTally
end
 tallies
read
 parameters

l
i
b
r
a
r
y
="v7-200n47g"

r
a
n
d
o
m
S
e
e
d
=00003
```

(continues on next page)

```
e
c
d7
b4
e3
e8
b
```

(continued from previous page)

```
p
e
r
B
a
t
c
h
=466000
b
a
t
c
h
e
s
=24

n
o
N
e
u
t
r
o
n
s
end
 parameters
```

The importance map defines two adjoint sources that correspond to the two tallies. Forward weighting, based on the response integrated over energy ("respWeighting"), is used. Because the true source is a point source, the subcell method of making a mesh source will fail, so the number of source trials is input. This number is small since the source is a monoenergetic point source. The Denovo calculations used the default S_8 quadrature and the P_3 Legendre order.

```
read
 importanceMap

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=1
```

(continues on next page)

(continued from previous page)

```
'   near detector

a
d
j
o
i
n
t
S
o
u
r
c
e 1

b
o
u
n
d
i
n
g
B
o
x 6 4  1
-1  21 19

u
n
i
t
=1
r
e
g
i
o
n
=2

r
e
s
p
o
n
s
e
I
D
=1
    end
 adjointSource
```

(continues on next page)

(continued from previous page)

```
'   far detector

a
d
j
o
i
n
t
S
o
u
r
c
e 2

b
o
u
n
d
i
n
g
B
o
x 7 3  2
-2  42 38

u
n
i
t
=1
r
e
g
i
o
n
=4

r
e
s
p
o
n
s
e
I
D
=1
    end
 adjointSource

r
e
s
p
w
e
i
g
```

(continues on next page)

(continued from previous page)

```
s
o
u
r
c
e
T
r
i
a
l
s
=100
end
 importanceMap

end
 data
end
```

Output

The results for the two region tallies, the first for the near detector and the second for the far detector after 60 minutes of computations (3 forward Denovo, 4 adjoint Denovo and 52 Monaco), were as follows.

```
Photon Region Tally 1.
                          average      standard     relat      FOM     stat checks
    tally/quantity         value       deviation    uncert    (/min)   1 2 3 4 5 6
    ------------------  -----------  -----------  -------  --------  -----------
    total flux (tl)      1.47918E+03  1.57461E+01  0.01065  1.70E+02  X - X X X X
    total flux (cd)      1.47936E+03  1.56963E+01  0.01061  1.71E+02  X - X - X X
    ------------------  -----------  -----------  -------  --------  -----------

 Photon Region Tally 2.
                          average      standard     relat      FOM     stat checks
    tally/quantity         value       deviation    uncert    (/min)   1 2 3 4 5 6
    ------------------  -----------  -----------  -------  --------  -----------
    total flux (tl)      4.57691E+01  2.81778E-01  0.00616  5.07E+02  X X X X X X
    total flux (cd)      4.57825E+01  2.80714E-01  0.00613  5.11E+02  X X X X X X
    ------------------  -----------  -----------  -------  --------  -----------
```

Note that both detectors have similarly low relative uncertainties (about 1%) even though the tally values differ by a factor of 30. These results should be compared to analog results (no biasing at all) and optimizations of each detector in separate input files, as shown in Table 1.22. The CADIS calculations for each detector (near or far) do exactly what they were supposed to do—optimize the Monte Carlo calculation for one tally or the other. The FOMs for the FW-CADIS calculation were about half of the FOMs for the single-detector CADIS calculations. Hence, for this two-detector problem, two CADIS calculations are just as efficient as one FW-CADIS calculation. For modern well-logging tools with up to a dozen detectors, a single FW-CADIS would be much more efficient and manageable. Note that the near detector still needs more time to pass the second (uncertainty fit) and the fourth (VOV fit) statistical checks. Neither of the single-detector CADIS calculations passed the fourth statistical check within an hour.

Fig. 1.23 shows a mesh tally of total photon flux in the y=0 plane for all four of the simulations: analog, CADIS for the near detector, CADIS for the far detector, and the FW-CADIS calculation for both.

Table 1.22: Comparison of different CADIS techniques for the litho-density problem

		Time		Near Detector			Far Detector		
		(min)		flux	relative	FOM	flux	relative	FOM
	For	Adj	MC	(/cm2/s)	uncert.	(/min)	(/cm2/s)	uncert.	(/min)
Analog			60.1	1.19E+03	0.3765	0.12	1.17E+02	0.7098	0.03
CADIS - Near		4.8	57.2	1.49E+03	0.0064	390	0.00E+00	0.0000	
CADIS - Far		4.7	57.0	8.28E+02	0.4162	0.09	4.56E+01	0.0048	703
FW-CADIS	2.8	4.4	52.1	1.48E+03	0.0107	149	4.58E+01	0.0062	444

/

1.5.4 AOS-100 using FW-CADIS and continuous-energy transport

The advanced variance reduction in MAVRIC can also be used when the final Monaco Monte Carlo transport calculation is performed using a CE cross section library. Simulations involving discrete-energy photon sources are best handled with CE. Consider the AOS-100, one of several radioactive material transport packaging systems developed by Alpha Omega Services, Inc., and a ^{60}Co source. (International Isotopes Inc. of Idaho Falls, Idaho, distributes the AOS Radioactive Material Transport Packaging Systems.)

A simple model of the AOS-100 package, which is constructed primarily of steel and tungsten, is shown in Fig. 1.24. The diameter is 71.12 cm, and the height is 91.44 cm. The innermost cylinder (16.51 cm diameter and 50.8 cm height) typically contains the material to be transported, but in this study, this region is simply modeled as an air region containing a uniform source of 1 Ci of ^{60}Co. This is conservative—it assumes the radioactive material containing the cobalt provides no self-shielding.

The objective in this study is to compute the dose rates around the cask. This can be done using a mesh tally. Note that the dose rates inside the package are not of concern—only the dose rates outside the package are.

The results of a 15-hour analog calculation (using only implicit capture with a lower weight limit of 10^{-7}) are shown in Fig. 1.25. This calculation does not show many photons that have escaped the package into the air, which is similar to reality for this heavily shielded cask. To compute dose rates outside the package, variance reduction is needed.

Input file

The sample problem file `mavric.aos100.inp` is located in the `samples\input` directory. For this demonstration, a very simplified geometry is used, with a few tungsten regions inside a steel cylinder. The library given at the beginning of the input is the MG library for the importance calculations. The final Monaco Monte Carlo calculation will use the CE library, which is specified in the parameters block. About 1 meter of air is modeled around the cask.

```
=mavric

A
O
S
-100
:
D
e
m
o
n
s
t
r
```

(continues on next page)

```
t
e
u
s
```

Fig. 1.23: Mesh tallies showing total photon flux in cm^2/s (left column) and its relative error (right column) in the y=0 plane.

Fig. 1.24: Simple AOS-100 cask geometry showing tungsten (brown) and steel (gray).

Fig. 1.25: Dose rates (mrem/hr/Ci) and relative uncertainties along the $y = 0$ midplane of the cask as calculated by an analog calculation.

(continued from previous page)

```
v7
-200
n47
g
read
 composition

s
s304            1    end

w
t
p
t
T
u
n
g
s
t
e
n     2  17
.8 4  74182 26 74183 14 74184 31 74186 29 end

d
r
y
-
a
i
r          3    end
end
 composition
```

(continues on next page)

(continued from previous page)

```
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

c
y
l
i
n
d
e
r 1  8
.255   25
.40
-25
.40

c
y
l
i
n
d
e
r 2 10
.795   27
.94
-27
.94

c
y
l
i
n
d
e
r 3 20
.955   27
.94
-27
.94

c
y
l
```

(continues on next page)

```
i
n
d
e
r 4 13
.335   40
.64  30
```

(continued from previous page)

```
c
y
l
i
n
d
e
r 5 13
.335
-30
.48
-40
.64

c
y
l
i
n
d
e
r 6 35
.56    45
.72
-45
.72


c
u
b
o
i
d  99  139
.7
-139
.7   139
.7
-139
.7  152
.4
-152
.4


m
e
d
i
a 3 1  1

m
e
d
i
a 1 1  2
-1
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a 2 1  3
-2

m
e
d
i
a 2 1  4

m
e
d
i
a 2 1  5

m
e
d
i
a 1 1  6
-3
-4
-5


m
e
d
i
a 3 1  99
-6

b
o
u
n
d
a
r
y 99
end
 geometry
```

In the definitions block, the photon dose response function, the cobalt-60 line spectrum, two grid geometries, and an energy boundaries structure are all defined. The first grid geometry is used for the deterministic calculation, the importance map, and the biased source. The second grid geometry is for the high-resolution (1 in.) mesh tally. The energyBounds defined here has a base structure of 30 bins that are 50 keV wide, with three bins that are 2 keV wide at the dominant cobalt line energies and the 511-keV annihilation gamma energy.

```
read
 definitions
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e 5

t
i
t
l
e
="ANSI standard (1977) neutron flux-to-dose-rate factors"

d
o
s
e
D
a
t
a
=9504
    end
 response


d
i
s
t
r
i
b
u
t
i
o
n 1

t
i
t
l
e
="cobalt-60 gammas/decay"

d
i
s
c
r
e
t
e   347140   826100 1173228 1332492  2158570    2505692 end
```

(continues on next page)

(continued from previous page)

```
t
r
u
e
p
d
f  0
.000075 0
.000076 0
.9985 0
.999826 0
.000012 0
.00000002 end
    end
 distribution



g
r
i
d
G
e
o
m
e
t
r
y 7

t
i
t
l
e
="mesh for discrete ordinates/importance map/biased source"

x
L
i
n
e
a
r 28
-35
.56  35
.56

y
L
i
n
e
a
r 28
-35
.56  35
.56
```

(continues on next page)

(continued from previous page)

```
z
L
i
n
e
a
r 36
-45
.72  45
.72


x
L
i
n
e
a
r 22
-139
.7  139
.7

y
L
i
n
e
a
r 22
-139
.7  139
.7

z
L
i
n
e
a
r 24
-152
.4  152
.4
    end
 gridGeometry


g
r
i
d
G
e
o
m
e
t
r
y 8
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="mesh for mesh tally - 1 inch voxels"

x
L
i
n
e
a
r  110
-139
.7   139
.7

y
L
i
n
e
a
r  110
-139
.7   139
.7

z
L
i
n
e
a
r  120
-152
.4   152
.4
    end
 gridGeometry


e
n
e
r
g
y
B
o
u
n
d
s 1

l
i
n
e
a
r 30 0
.00
```

(continues on next page)

(continued from previous page)

```
b
o
u
n
d
s  0
.510
e
+6 0
.512
e
+6   1
.172
e6 1
.174
e6   1
.331
e6 1
.333
e6 end
    end
 energyBounds
end
 definitions
```

The source is modeled as a uniform volumetric source in the center region of the cask. Because the distribution of cobalt gamma rays was entered as gammas per decay, the keyword "useNormConst" will set the source strength to be the total of the energy distribution—about 2 photons/decay. The "multiplier" keyword is used to multiply that strength by 37e9 decays/sec to get 1 Ci.

```
read
 sources

s
r
c 1

t
i
t
l
e
="one Ci of cobalt-60"

u
s
e
N
o
r
m
C
o
n
s
t
```

(continues on next page)

(continued from previous page)

```
m
u
l
t
i
p
l
i
e
r=37e9

c
y
l
i
n
d
e
r  8
.255   25
.40
-25
.40

p
h
o
t
o
n
s

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources
```

A single mesh tally is defined and is limited to the air region outside of the cask. A multiplier of 1,000 is used to convert the response values from rem/hr to mrem/hr.

```
read
 tallies

m
e
s
h
T
a
l
l
y 1

p
h
o
t
o
n

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=8

r
e
s
p
o
n
s
e
I
D
=5

u
n
i
t
=1
r
e
g
i
o
```

(continues on next page)

```
n
=7
```

(continued from previous page)

```
e
n
e
r
g
y
B
o
u
n
d
s
I
D
=1
    end
 meshTally


m
u
l
t
i
p
l
i
e
r
=1000
.0
end
 tallies
```

In this problem, the importance calculations will use the 200/47 MG library, which will transport all particles contained in the library by default. The keyword "noNeutrons" is used to turn off neutron transport during the Denovo calculations, thereby saving time. The final Monaco calculation will use the CE library ("ceLibrary="), which only transports the particles specifically requested by the user (to avoid loading large amounts of cross section from disk to memory). Thus, the keyword "photons" is included to specifically tell the CE Monaco to transport photons.

```
read
 parameters

r
a
n
d
o
m
S
e
e
d
=00003
e
c
```

(continues on next page)

```
d7
b4
e3
e8
b
```

(continued from previous page)

```
c
e
L
i
b
r
a
r
y
="ce_v7np_endf.xml"

p
e
r
B
a
t
c
h
=2000000
b
a
t
c
h
e
s
=233

p
h
o
t
o
n
s
n
o
N
e
u
t
r
o
n
s
end
 parameters
```

The importance map uses FW-CADIS to construct a map and biased source that will optimize the photon dose rate in the air outside the cask. Since photon scatter is typically forward peaked, an S_{12} quadrature and P_5 Legendre scattering expansion are used.

```
read
 importanceMap
```

(continues on next page)

(continued from previous page)

```
a
d
j
o
i
n
t
S
o
u
r
c
e 1

b
o
u
n
d
i
n
g
B
o
x 139
.7
-139
.7   139
.7
-139
.7  152
.4
-152
.4

u
n
i
t
=1
r
e
g
i
o
n
=7

r
e
s
p
o
n
s
e
I
D
=5
```

(continues on next page)

(continued from previous page)

```
    end
 adjointSource

r
e
s
p
W
e
i
g
h
t
i
n
g


g
r
i
d
G
e
o
m
e
t
r
y
I
D
=7

m
a
c
r
o
m
a
t
e
r
i
a
l

m
m
T
o
l
e
r
a
n
c
e
=0
.01
```

(continues on next page)

(continued from previous page)

```
    end
 macromaterial


q
u
a
d
r
a
t
u
r
e
=12

l
e
g
e
n
d
r
e
=5
end
 importanceMap
```

Output file

Results for the mesh tally after 958 minutes (27 forward Denovo, 31 adjoint Denovo, and 900 CE-Monaco) are shown in Fig. 1.26. Since dose rates inside the package are not of concern, that region was excluded from the mesh tally. Due to the optimization that focused the Monte Carlo calculation on dose rates outside the cask, values of the dose rate inside the cask are underestimated and should not be used. Also note that voxels along the outer cylindrical edge of the package could show low dose rates, since the voxel value is an average and only part of the voxel is actually outside the package. The resolution of the mesh tally is 2.54 cm.

The flux using the user-defined energy bin boundaries for a point 10 cm above the top of the package (along the axis) is shown in Fig. 1.27. Note that since the importance map was made to optimize the photon dose rate, some of the low-energy bins that do not contribute much to dose may have larger uncertainties.

Fig. 1.28 and Fig. 1.29 show the ratios of the dose rates computed using a MG calculation to the CE calculation. Dose rates inside the cask should not be compared because the importance map is focused on dose outside the cask, so low-energy photons are not simulated inside. The 47-group MG calculation is fairly close to the CE-calculation in dose rate (10% high axially, 20% high radially), but the 19-group MG dose rates are much higher than the CE. Neither of the MG calculations shows the 1.17 and 1.33 MeV lines in the energy spectra.

Fig. 1.26: Dose rates (mrem/hr/Ci) and relative uncertainties from the CE FW-CADIS calculation showing the mid-plane views of the cask ($z = 0$ above and $y = 0$ below).

Fig. 1.27: Flux 10 cm above the cask.

Fig. 1.28: Ratio of the 47-group MG computed dose rates to the CE dose rates ($y = 0$ left and $z = 0$ right).

Fig. 1.29: Ratio of the 19-group MG computed dose rates to the CE dose rates ($y = 0$ left and $z = 0$ right).

1.5.5 Independent spent fuel storage installation

A good example of a problem in which the dose rate needs to be known well everywhere——in low dose areas and high dose areas——is an independent spent fuel storage installation. The dose rates around these arrays of spent fuel casks need to be evaluated over a large area of ground to determine the boundary of the controlled area. This sample problem uses a simplified model of a cask array, shown in Fig. 1.30 and Fig. 1.31, to demonstrate the FW-CADIS method for obtaining the dose rates with reasonably low relative uncertainties over a mesh tally which covers a very large area.

Fig. 1.30: Array of eight casks.

Fig. 1.31: Cask detail.

Source term

The calculation of the spent fuel source term using data from the Kewaunee nuclear power plant is described in the cask example problem and is modeled in the first part of `mavric.isfsi.inp` with ORIGEN. The result of this calculation is a binary concentration (ft71f001) file. This file also contains a list of the group-wise neutron source term ("total neutron spectra, neutrons/sec/basis") and photon source term ("gamma spectra, photons/sec/basis") for each time step. In this example problem, the source term for the MAVRIC calculation will be read directly from the binary concentration file. The file contains the concentration and source-term data at each of 64 time steps. For this analysis, the photon source at the last time step will be used.

Input file

The following is a listing of the second part (the MAVRIC input) of the file `mavric.isfsi.inp` located in the SCALE `samples\input` directory. Note that soil and air are included in the model to properly account for dose near the ground. The mesh tally does not extend into the air above 2 meters since this problem is only concerned with the area near the ground where people could be. For MAVRIC to read the ORIGEN binary concentration file, it must be named as a Fortran unit file with a number matching the distribution input. In this example, unit 71 is used in both the ORIGEN input and MAVRIC input.

```
=mavric

I
S
F
S
I
-
f
o
r
w
a
r
d
-
w
e
i
g
h
t
```

(continues on next page)

```
d
a
d
j
```

(continued from previous page)

```
v7
-27
n19
g
```

The materials include the fresh fuel (with a density representing homogenization), concrete, steel, air, and ordinary soil.

```
read
 composition

w
t
p
t
F
u
e
l   1 0
.913717475 18         6000  0
.00939719    7014  0
.00528993
                    8016  9
.73397641   13000  0
.00715715   14000  0
.01031670
                   15000  0
.02227505   22000  0
.00780567   24000  0
.36655141
                   25000  0
.01716839   26000  0
.72041451   27000  0
.00523824
                   28000  0
.68955526   40000 15
.78990702   41000  0
.05130153
                   42000  0
.02844690   50118  0
.25877903   92235  3
.03560962
                   92238 69
.24080999
                 1
.0 293
.0 end

o
r
c
o
n
c
r
e
t
e 2 1
.0 293
.0 end
```

(continues on next page)

(continued from previous page)

```
s
s304      3 1
.0 293
.0 end

d
r
y
-
a
i
r    4 1
.0 293
.0 end

w
t
p
t
S
o
i
l   5 1
.685 12  1000 3
.498   6000  2
.138   8016 60
.826  11000 0
.579
                          13000 7
.489  14000 18
.841  17000  0
.026  19000 0
.582
                          20000 0
.896  22000  0
.488  25000  0
.097  26000 4
.540
                 1
.0 293
.0 end
end
 composition
```

The geometry models one cask and then repeats the cask model eight times using an array.

```
read
 geometry

u
n
i
t  1

z
c
y
l
i
n
d
e
r  1   90
```

(continues on next page)

(continued from previous page)

```
z
c
y
l
i
n
d
e
r  2   90
.0  240
.6
-240
.6

z
c
y
l
i
n
d
e
r  3   90
.0  280
.6
-280
.6

z
c
y
l
i
n
d
e
r  4   95
.0  280
.6
-280
.6

z
c
y
l
i
n
d
e
r  5  100
.0  280
.6
-280
.6

z
c
y
l
i
n
d
```

(continues on next page)

(continued from previous page)

```
z
c
y
l
i
n
d
e
r  7  170
.0  280
.6
-280
.6

z
c
y
l
i
n
d
e
r  8  170
.0  285
.6
-285
.6

c
u
b
o
i
d    11  170  90 30
-30   280
.6 255
.6

c
u
b
o
i
d    12  30
-30 170 90    280
.6 255
.6

c
u
b
o
i
d    13
-90
-170 30
-30  280
.6 255
.6
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d    14  30
-30
-90
-170  280
.6 255
.6

c
u
b
o
i
d    21  170  90 30
-30
-255
.6
-280
.6

c
u
b
o
i
d    22  30
-30 170 90
-255
.6
-280
.6

c
u
b
o
i
d    23
-90
-170 30
-30
-255
.6
-280
.6

c
u
b
o
i
d    24  30
-30
-90
-170
-255
.6
-280
.6
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d    99  340
.0
-340
.0   340
.0
-340
.0   285
.6
-285
.6


m
e
d
i
a  1    1   1

m
e
d
i
a  3    1   2
-1

m
e
d
i
a  2    1   3
-2

m
e
d
i
a  4    1   4
-3

m
e
d
i
a  3    1   5
-4
-11
-12
-13
-14
-21
-22
-23
-24
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  2    1   6
-5
-11
-12
-13
-14
-21
-22
-23
-24

m
e
d
i
a  3    1   7
-6
-11
-12
-13
-14
-21
-22
-23
-24

m
e
d
i
a  3    1   8
-7

m
e
d
i
a  4    1   11
-4 7

m
e
d
i
a  4    1   12
-4 7

m
e
d
i
a  4    1   13
-4 7
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  4    1   14
-4 7

m
e
d
i
a  4    1   21
-4 7

m
e
d
i
a  4    1   22
-4 7

m
e
d
i
a  4    1   23
-4 7

m
e
d
i
a  4    1   24
-4 7

m
e
d
i
a  4    1   99
-8

b
o
u
n
d
a
r
y 99

g
l
o
b
a
l
u
n
i
t 2
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d 1   1360
-1360      680
-680       571
.2    0
.0

c
u
b
o
i
d 2   2040
-2040     1360
-1360        0
.0
-60
.0

c
u
b
o
i
d 3  12000
-12000   12000
-12000       0
.0
-100
.0

c
u
b
o
i
d 4  12000
-12000   12000
-12000   10000
.0
-100
.0

a
r
r
a
y 10 1
p
l
a
c
e 1 1 1
-1020
-340 285
.0
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  2  1   2

m
e
d
i
a  5  1   3
-2

m
e
d
i
a  4  1   4
-3
-1

b
o
u
n
d
a
r
y 4
end
 geometry

read
 array

a
r
a
=10
n
u
x
=4
n
u
y
=2
n
u
z
=1
f
i
l
l 1 1 1 1   1 1 1 1   end
 fill
```

(continues on next page)

(continued from previous page)

```
end
 array
```

The definitions block contains the photon dose response, a mesh geometry for the discrete-ordinates calculations, a uniform mesh for the mesh tally, and the photon energy distribution read from the binary concentration file (located on unit 71, the last time step case 64).

```
read
 definitions

r
e
s
p
o
n
s
e 6

s
p
e
c
i
a
l
D
o
s
e
=9504
    end
 response

g
r
i
d
G
e
o
m
e
t
r
y 3

t
i
t
l
e
="exercise geometry 68x44x24 = 71808"

x
p
l
```

(continues on next page)

```
a
n
e
s
-12000
-10000
-8000
```

(continued from previous page)

```
-2040
-1870
-1700
-1530

-1360
-1275
-1190
-1150
-1110
-1070
-1020
-970
-930
-890
-850
-765

-680
-595
-510
-470
-430
-390
-340
-290
-250
-210
-170
-85
                0 85 170 210 250 290 340 390 430 470 510 595 680
                765 850 890 930 970 1020 1070 1110 1150 1190 1275 1360
                1530 1700 1870 2040
                3000 4000 6000 8000 10000 12000 end

y
p
l
a
n
e
s
-12000
-10000
-8000
-6000
-4000
-2000

-1360
-1190
-1020
-850

-680
-595
-510
-470
-430
-390
-340
-290
-250
```

(continues on next page)

(continued from previous page)

```
                0 85 170 210 250 290 340 390 430 470 510 595 680
                850 1020 1190 1360
                2000 4000 6000 8000 10000 12000 end

z
p
l
a
n
e
s
-100
-50
-30
-15 0 25 50 75 100 200 300 400 500 570 600 800
                900 1000 1500 2000 3000 4000 6000 8000 10000 end
    end
 gridGeometry

g
r
i
d
G
e
o
m
e
t
r
y 4

t
i
t
l
e
="large voxels for mesh tally"

x
L
i
n
e
a
r 24
-12000
.0 12000
.0

y
L
i
n
e
a
r 24
-12000
.0 12000
.0
```

(continues on next page)

(continued from previous page)

```
z
L
i
n
e
a
r  1      0
.0   200
.0
    end
 gridGeometry


d
i
s
t
r
i
b
u
t
i
o
n 1
'       use result from kewaunee.origen.inp, case 64, master photon library

s
p
e
c
i
a
l
="origensBinaryConcentrationFile"

f
i
l
e
n
a
m
e
=
"
f
t71
f001
"

p
a
r
a
m
e
t
e
r
s 71 64 4 end
```

(continues on next page)

(continued from previous page)

```
    end
 distribution
end
 definitions
```

The source can be defined in two ways. Since there are eight casks, eight sources could be defined, each over a cylinder with a strength of 7.155×10^{16} photon/s. In this example of eight identical sources, one source region can be defined and then limited to only exist in the spent fuel material (the first material) but with a strength for all the casks of 5.724×10^{17} photon/s.

```
read
 sources

s
r
c 1

t
i
t
l
e
="each cask holds 1/6 of kewaunee core"

s
t
r
e
n
g
t
h=5.724e17

c
u
b
o
i
d
-1115 1115  435
-435  514
.2  57

m
i
x
t
u
r
e
=1

p
h
o
t
o
```

(continues on next page)

```
n
s
```

(continued from previous page)

```
e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources
```

The mesh tally covers only the first 2 meters above the ground since the dose rate above that would not impact a person.

```
read
 tallies

m
e
s
h
T
a
l
l
y 1

t
i
t
l
e
="120m from cask array center"

p
h
o
t
o
n

g
r
i
d
G
e
o
m
e
t
r
y
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e
I
D
=6
    end
 meshTally
end
 tallies

'------------------------------------------------------------------------------
' Parameters Block
'------------------------------------------------------------------------------
read
 parameters

r
a
n
d
o
m
S
e
e
d
=8655740521000041

p
e
r
B
a
t
c
h
=940000
b
a
t
c
h
e
s
=60
end
 parameters
```

The adjoint source is placed everywhere that the dose rate is desired——near the ground but not very close to or in between the casks (where people will not be). The macro material option is used here to ensure that the discrete-

ordinates calculation is more representative of the problem.

```
read
 importanceMap

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=3

a
d
j
o
i
n
t
S
o
u
r
c
e 1

b
o
u
n
d
i
n
g
B
o
x 12000
-12000   12000
-12000  600
.0 0
.0

r
e
s
p
o
n
s
e
I
D
=5
```

(continues on next page)

(continued from previous page)

```
u
n
i
t
=2
r
e
g
i
o
n
=3
    end
 adjointSource

r
e
s
p
W
e
i
g
h
t
i
n
g

m
a
c
r
o
m
a
t
e
r
i
a
l

m
m
T
o
l
e
r
a
n
c
e
=0
.001
```

(continues on next page)

(continued from previous page)

```
    end
 macromaterial

s
a
v
e
E
x
t
r
a
M
a
p
s
end
 importanceMap

end
 data
end
```

Output

The MAVRIC calculational times were 3 minutes for the forward Denovo, 3.5 minutes for the adjoint Denovo, and 60 minutes for the Monaco forward Monte Carlo. Results for the mesh tally of dose rates are shown in Fig. 1.32. For a longer Monaco calculation (64 hr), the mesh tally results are shown in Fig. 1.33. Note that the scale for the dose rate has been adjusted to only show the values outside of the cask array.

Using the Mesh File Viewer, the distribution of relative uncertainty in a mesh tally can be plotted. For this 1 hr calculation, 50% of the voxels in the mesh tally had less than 20% relative uncertainty. Fig. 1.34 shows how the distribution of relative errors changes with longer run times. For the 64 hr run, 90% of the voxels had less than 10% relative uncertainty.

Fig. 1.32: Photon dose rate values in rem/hr (left) and the relative uncertainty (right) for the area around the cask array (1 hr Monaco).

Fig. 1.33: Photon dose rate values in rem/hr (left) and the relative uncertainty (right) for the area around the cask array (64 hr Monaco). For the uncertainty plot, purple represents <=5%.

Fig. 1.34: Distribution of relative uncertainties for different run times of `mavric.isfsi.inp` showing the fraction of the mesh tally voxels that had less than a given amount of relative uncertainty.

1.5.6 TN24-P spent fuel cask

For an example that uses multiple sources, user-defined distributions in those sources, macromaterials for improved S_N calculations, and the automated variance reduction capabilities in MAVRIC, consider the model for the TN-24P cask, as used in previous SCALE shielding reports [WDP+09] and shown in Fig. 1.35. This model contains two types of PWR spent fuel assemblies (Types V and W, both Westinghouse 15×15 assemblies of different starting enrichments and burnups), each with specified neutron and photon sources, in an aluminum/boron fuel basket. The cask is made of forged steel for photon shielding with a resin layer for neutron shielding. The model also includes three activated hardware regions (bottom nozzle, top nozzle, and top plenum), which consist of specified amounts of ^{60}Co (a photon source). The task for this example is to calculate the total dose rate within 2 meters of the cask surface.

Fig. 1.35: MAVRIC model of the TN24-P cask. Materials: spent fuel (light and dark yellow), steels (blues), resin (green), and other metals (gray).

For MAVRIC, this means that the calculation of a dose rate mesh tally is calculated using FW-CADIS to ensure that each voxel has low relative uncertainty, independent of the dose rate. Without MAVRIC, the calculation of dose rate everywhere in three dimensions would be too challenging. Most likely, the dose rate would be evaluated with reasonable uncertainty at only a few locations. In fact, with analog calculations, this example would be a very difficult problem since most source particles never leave the cask, just as in the real-life situation. This type of problem really benefits from the CADIS-biased source distribution, in which source particles deep inside the cask are sampled very rarely since they do not contribute significantly to the response.

Input file

The following is a partial list of the file `mavric.tn24p.inp` located in the SCALE `samples\input` directory. This calculation will use the coarse-group shielding library for all of the importance map calculations but then will use the fine-group library for the final Monaco step. The full geometry and source distributions are not printed here due to their length.

```
=mavric

M
o
n
a
c
o
/
M
A
V
R
I
C
T
r
a
i
n
i
n
g
-
E
x
e
r
c
i
s
e 3
.
G
r
a
p
h
i
t
e
S
h
i
e
l
d
i
n
g
M
e
a
s
u
r
e
m
```

(continues on next page)

(continued from previous page)

```
v7
-27
n19
g
read
 composition

...
end
 composition

read
 geometry

...
end
 geometry

read
 array

...
end
 array
```

The definitions block includes three responses (neutron, photon, total), two grid geometries (one for the importance map calculations and one for a mesh tally), one cylindrical mesh for a mesh tally, five distributions for the energy spectra of the sources, and two distributions for the spatial distributions of the fuel assembly sources.

```
read
 definitions

r
e
s
p
o
n
s
e 1
s
p
e
c
i
a
l
D
o
s
e
=9029  end
 response

r
e
s
p
o
n
s
e 2
s
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e 3
s
p
e
c
i
a
l
D
o
s
e
=9729  end
 response


g
r
i
d
G
e
o
m
e
t
r
y 1

t
i
t
l
e
="for discrete ordinates calculations  48 x 48 x 61"

...
    end
 gridGeometry

g
r
i
d
G
e
o
m
e
t
r
y 2
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="for mesh tallies"

x
L
i
n
e
a
r 66
-330 330

y
L
i
n
e
a
r 66
-330 330

z
L
i
n
e
a
r 90
-435 465
    end
 gridGeometry

c
y
l
G
e
o
m
e
t
r
y 3

r
a
d
i
u
s
L
i
n
e
a
r 66 0 330
```

(continues on next page)

(continued from previous page)

```
d
e
g
r
e
e
L
i
n
e
a
r 72 0 360

z
L
i
n
e
a
r 90
-435 465
    end
 cylGeometry


d
i
s
t
r
i
b
u
t
i
o
n 1

t
i
t
l
e
="neutron energy distribution for W assembly"

a
b
s
c
i
s
s
a
... end

t
r
u
e
P
D
F
... end
```

(continues on next page)

(continued from previous page)

```
    end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 2

t
i
t
l
e
="photon energy distribution for W assembly"

a
b
s
c
i
s
s
a
... end

t
r
u
e
P
D
F
... end
    end
 distribution



d
i
s
t
r
i
b
u
t
i
o
n 3
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="neutron energy distribution for V assembly"

a
b
s
c
i
s
s
a
... end

t
r
u
e
P
D
F
... end
    end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 4

t
i
t
l
e
="photon energy distribution for V assembly"

a
b
s
c
i
s
s
a
... end
```

(continues on next page)

(continued from previous page)

```
t
r
u
e
P
D
F
... end
    end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 5

t
i
t
l
e
="cobalt-60 gammas/decay"

s
p
e
c
i
a
l
="origensDiscreteGammas"

p
a
r
a
m
e
t
e
r
s 27 60 end
    end
 distribution


d
i
s
t
r
i
b
u
t
```

(continues on next page)

(continued from previous page)

```
d
i
s
t
r
i
b
u
t
i
o
n 102
s
p
e
c
i
a
l
="pwrGammaAxialProfile"   end
 distribution


r
u
n
S
a
m
p
l
e
T
e
s
t
s
m
a
k
e
C
h
a
r
t
s
end
 definitions
```

Seven sources are defined——a neutron and photon source for each type of fuel assembly, and three activated hardware regions.

```
read
 sources
```

(continues on next page)

(continued from previous page)

```
s
r
c 1

t
i
t
l
e
="W assembly, neutron source"

n
e
u
t
r
o
n
s

s
t
r
e
n
g
t
h=1.6472e9

z
C
y
l
i
n
d
e
r 71
.0  182
.9
-182
.9

z
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=101
z
S
c
a
```

(continues on next page)

(continued from previous page)

```
m
i
x
t
u
r
e
=2

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src

s
r
c 2

t
i
t
l
e
="W assembly, photon source"

p
h
o
t
o
n
s

s
t
r
e
n
g
t
h=5.3638e16
```

(continues on next page)

```
z
C
y
l
i
n
d
```

(continued from previous page)

```
z
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=102
z
S
c
a
l
e
D
i
s
t

m
i
x
t
u
r
e
=2

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=2
    end
 src
```

(continues on next page)

```
s
r
c 3
```

(continued from previous page)

```
t
i
t
l
e
="V assembly, neutron source"

n
e
u
t
r
o
n
s

s
t
r
e
n
g
t
h=7.1927e8

z
C
y
l
i
n
d
e
r 63
.0  182
.9
-182
.9

z
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=101
z
S
c
a
l
e
D
i
```

(continues on next page)

(continued from previous page)

```
m
i
x
t
u
r
e
=12

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=3
    end
 src

s
r
c 4

t
i
t
l
e
="V assembly, photon source"

p
h
o
t
o
n
s

s
t
r
e
n
g
t
h=1.8234e16
```

(continues on next page)

```
z
C
y
l
i
n
d
```

(continued from previous page)

```
z
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=102
z
S
c
a
l
e
D
i
s
t

m
i
x
t
u
r
e
=12

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=4
    end
 src

s
r
c 6
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="bottom nozzel Co-60 source"

p
h
o
t
o
n
s

s
t
r
e
n
g
t
h=1.7960e14

z
C
y
l
i
n
d
e
r 71
.0
-186
-193

m
i
x
t
u
r
e
=9

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=5
```

(continues on next page)

(continued from previous page)

```
    end
 src


s
r
c 7

t
i
t
l
e
="top nozzle Co-60 source"

p
h
o
t
o
n
s

s
t
r
e
n
g
t
h=1.0103e14

z
C
y
l
i
n
d
e
r 71
.0 212
.8 203
.9

m
i
x
t
u
r
e
=10

e
D
i
s
t
r
i
b
u
t
```

(continues on next page)

(continued from previous page)

```
    end
 src


s
r
c 8

t
i
t
l
e
="plenum Co-60 source"

p
h
o
t
o
n
s

s
t
r
e
n
g
t
h=6.3137e13

z
C
y
l
i
n
d
e
r 71
.0 201
.0 182
.9

m
i
x
t
u
r
e
=11

e
D
i
s
t
r
i
b
u
t
```

(continues on next page)

(continued from previous page)

```
    end
 src
end
 sources
```

Four mesh tallies are used to collect the neutron dose rate, the photon dose rate, and the total dose rate.

```
read
 tallies

m
e
s
h
T
a
l
l
y 1

n
e
u
t
r
o
n

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=2

r
e
s
p
o
n
s
e
I
D
=1

n
o
G
r
o
u
p
F
```

(continues on next page)

(continued from previous page)

```
 end
 meshTally

m
e
s
h
T
a
l
l
y 2

p
h
o
t
o
n

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=2

r
e
s
p
o
n
s
e
I
D
=2

n
o
G
r
o
u
p
F
l
u
x
e
s
```

(continues on next page)

(continued from previous page)

```
 end
 meshTally

m
e
s
h
T
a
l
l
y 11

n
e
u
t
r
o
n

c
y
l
G
e
o
m
e
t
r
y
I
D
=3

r
e
s
p
o
n
s
e
I
D
=1

n
o
G
r
o
u
p
F
l
u
x
e
s
```

(continues on next page)

(continued from previous page)

```
 end
 meshTally

m
e
s
h
T
a
l
l
y 12

p
h
o
t
o
n

c
y
l
G
e
o
m
e
t
r
y
I
D
=3

r
e
s
p
o
n
s
e
I
D
=2

n
o
G
r
o
u
p
F
l
u
x
e
s
```

(continues on next page)

(continued from previous page)

```
 end
 meshTally
end
 tallies
```

The goal of this example is to calculate the total dose outside the cask. Therefore, the adjoint source uses the total dose rate response function for its energy component, whereas for the spatial component, it uses a large block around the cask. Note the "mixture=" keyword, which restricts the adjoint source to only exist where the material is air (13). There is no need to put adjoint source deep in the cask since the dose rates inside the cask are not of interest. Response weighting is used to put more adjoint source in the low dose areas outside the cask. Note that since this area is air, not many interactions/scatter take place, so a great balance in relative uncertainties near and far from the cask should not be expected. Macromaterials are used to improve the results from the discrete-ordinates calculations, which should improve the FOM of the final Monaco calculation. The geometry images in *Macromaterials for SN geometries* are taken from this problem.

```
read
 importanceMap

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=1

a
d
j
o
i
n
t
S
o
u
r
c
e 1

b
o
u
n
d
i
n
g
B
o
x  330
-330  330
-330  465
-435
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e
I
D
=3

m
i
x
t
u
r
e
=13
    end
 adjointSource

r
e
s
p
W
e
i
g
h
t
i
n
g

r
e
d
u
c
e

s
u
b
C
e
l
l
s
=3

m
a
c
r
o
m
a
t
e
```

(continues on next page)

(continued from previous page)

```
m
m
T
o
l
e
r
a
n
c
e
=0
.001
    end
 macromaterial
end
 importanceMap

end
 data
end
```

Output

The distributions used by the source descriptions of the TN24-P model are shown in Fig. 1.37, and the responses used in this problem are shown in Fig. 1.36. Fig. 1.38 and Fig. 1.39 show the total (neutron + photon) dose rate outside the TN24-P cask, up to 2 meters from each surface using rectilinear and cylindrical mesh tallies with 10 cm voxels. Uncertainties in the computed dose rates were 3–4% after this 16 hr calculation. The scale of the figure was adjusted to only show the dose rate outside the cask; dose rates inside the cask went as high as 6×10^5 rem/hr. Likewise, the scale of the uncertainties ranged from 0 to 10% to highlight the uncertainties outside the cask. Relative uncertainties inside the cask were much higher (white areas) since those areas were deemed unimportant by the chosen adjoint source. Obtaining dose rates on a 10 cm mesh would not be achievable without the variance reduction capabilities of MAVRIC.

Fig. 1.36: Neutron (left) and photon (right) dose rate response functions.

Fig. 1.37: Distributions in the TN24-P model.

Fig. 1.38: Rectilinear mesh tally of total dose rate (rem/hr) and its relative uncertainty along the x=0 plane.

Fig. 1.39: Cylindrical mesh tally of total dose rate (rem/hr) and its relative uncertainty along the =0° plane.

CHAPTER

TWO

MAVRIC APPENDIX A: CAAS CAPABILITY

2.1 Introduction

Modeling criticality accident alarm systems (CAAS) presents challenges since the analysis consists of both a criticality problem and a deep-penetration shielding problem [PPJ09][PLMP10]. Modern codes are typically optimized to handle one of those types of problems but usually not both. The two problems also differ in scale—the criticality problem depends on materials relatively close to the fissionable materials while the shielding problem can cover a much larger range. SCALE now contains fully three-dimensional tools to perform both parts of a CAAS analysis.

CAAS analysis can be performed with SCALE using the KENO-VI criticality code and the MAVRIC shielding sequence. First, the fission distribution (in space and energy) is determined by KENO-VI. This distribution is saved to a file using a user-specified three-dimensional mesh grid and an energy structure from the cross section library (or a user-defined energy structure). MAVRIC then uses the fission distribution as the source for a shielding calculation. MAVRIC is designed to implement advanced variance reduction methods to calculate dose rates or detector responses for difficult shielding problems.

For different types of shielding and different combinations of sources and detector locations, different strategies can be used within SCALE [PW12][WODonnellN12]. Due to the way that cross sections for neutron reactions that create photons are stored in ENDF, some of the parameters used in the CAAS capability have changed since SCALE 6.1. Please be sure to understand and follow the new guidance for the correct accounting of secondary photons from neutron reactions [MP13b][MP13c][MP13a].

2.2 Methods

The CAAS capability in SCALE is a two-step approach using KENO-VI and MAVRIC. The first step is the determination of the source distribution, done with the CSAS6 sequence which uses the KENO-VI functional module. Along with calculating the system k_{eff}, KENO-VI has been modified to now accumulate the fission distribution over the non-skip generations. This information is collected on a three-dimensional Cartesian mesh that overlays the physical geometry model and is saved as a Monaco mesh tally file. A utility program is used to convert the mesh tally into a Monaco mesh source.

The mesh source is then used in the second step as the source term in MAVRIC. The absolute source strength is set by the user based on the total number of fissions (based on the total power released) during the criticality excursion. Further neutron multiplication should be prevented in the MAVRIC transport calculation. Because the fission neutrons have already been accounted for in the KENO-VI calculation, failure to suppress neutron multiplication in the MARVIC sequence would lead to incorrect flux estimates. In addition, if further fissions were allowed, Monaco would add neutrons to its particle bank faster than they could be removed (since the system is at or above critical) and the simulation may never finish.

For the transport part of a CAAS analysis, MAVRIC can be optimized to calculate one specific detector response at one location using CADIS or can be optimized to calculate multiple responses/locations with roughly the same relative

uncertainty using FW-CADIS. For calculating mesh tallies of fluxes or dose rates, MAVRIC also uses FW-CADIS to help balance the Monaco Monte Carlo calculation such that low flux voxels are computed with about the same relative uncertainty as high flux voxels.

With this two-step approach, users will have a great deal of flexibility in modeling CAAS problems. The CSAS6 step and the MAVRIC step could both use the same geometry and materials definitions or could have different levels of detail included in each. The fission source distribution from one CSAS6 calculation could be used in a number of different MAVRIC building/detector models, with each MAVRIC calculation being optimized for a given type of detector.

2.3 User Input

The user can create either one input file containing both the CSAS6 and MAVRIC calculations or can create two input files—one for each sequence. The materials and geometry for these two models could be the same but do not have to be. For example, the CSAS6 sequence might only contain the materials and geometry important to the criticality calculation. Note, however, that the critical source geometry and materials should be modeled identically in both problems. This allows users greater flexibility in modeling their specific problems.

2.3.1 KENO-VI input

For the criticality problem, the only extra input a user needs to supply is the keyword "cds=yes" in the parameter block and a spatial mesh around all of the fissionable materials of the problem in its own gridGeometry block. Standard input for KENO-VI is described in the KENO-VI chapter and CSAS6 chapter. The mesh used for the fission source distribution is input using the "read gridGeometry *id*" block, where *id* is an identification number for that grid. Note that only one grid can be specified, but that may change in the future. The cells of the mesh are specified in each dimension separately by either (1) listing all of the planes bounding the cells (keyword "xplanes" followed by an "end"), (2) using keyword "xLinear n a b" to specify n cells between a and b, or by (3) specifying the minimum plane, the maximum plane, and how many cells to make in that dimension ("xmin=", "xmax=", "numXCells="). The keywords "xplanes" and "xLinear" can be used together and multiple times. Similar keywords are used for the y- and z-dimensions. An example CSAS6 input file that collects the fission distribution information would be as follows:

```
=csas6

C
A
A
S
E
x
a
m
p
l
e

v7
-238
n
read
 composition

...
end
 composition
```

(continues on next page)

(continued from previous page)

```
read
 parameters

...

c
d
s
=
y
e
s
end
 parameters
read
 geometry

...
end
 geometry
read
 gridGeometry

1

t
i
t
l
e
="Mesh for Collecting Fission Source"

x
L
i
n
e
a
r 13 0
.0 78
.0

y
p
l
a
n
e
s 0 8 16 24 32 34 36 38 40 48 56 64 72 end

z
L
i
n
e
a
r 10
-2
.54 77
.46
```

(continues on next page)

(continued from previous page)

```
end
 gridGeometry
end
 data
end
```

The fission source distribution collected by KENO-VI is saved to a Monaco mesh tally file and copied back to the home area with the name "*problemName*.fissionSource.3dmap". This file can be viewed with the Mesh File Viewer capability of Fulcrum that comes with SCALE. Note that the finer the mesh spacing is the more generations/histories will have to be simulated by the criticality calculation in order to reduce the stochastic uncertainty in each mesh voxel of the distribution. Regardless of the mesh size, creation of a fission mesh source file will take more iterations than the number required to find k_{eff}. KENO-VI also saves the value of the system the average number of neutrons per fission, in a file called "*problemName*.kenoNuBar.txt". This value is needed to properly determine the source strength.

2.3.2 Mesh tally to mesh source conversion

A utility program is used to convert the Monaco mesh tally file into a Monaco mesh source file. It can be part of the CSAS6 input file. The user then needs to copy the resulting *.msm file back to his home area.

```
=csas6

...
end

=mt2msm
'fissionSource.3dmap'    ! existing Keno fission source mesh tally
1
!
w
h
i
c
h
f
a
m
i
l
y
(
f
o
r
K
e
n
o
f
i
l
e
s
,
t
h
```

(continues on next page)

```
e
r
e
1
s
o
n
```

(continued from previous page)

```
-1
!
u
s
e
t
h
e
w
h
o
l
e
f
a
m
i
l
y
(
k
e
e
p
a
l
l
e
n
e
r
g
y
g
r
o
u
p
s
)
1
!
p
a
r
t
i
c
l
e
t
y
p
e
f
o
r
*
```

(continues on next page)


```
m
s
m
f
```

(continued from previous page)

```
'fissionSource.msm'      ! name of newly created mesh source map file
end

=shell

c
o
p
y
f
i
s
s
i
o
n
S
o
u
r
c
e
.
m
s
m
"
C
:
\
m
y
d
o
c
u
~1
\
c
a
a
s
E
x
a
m
p
l
e
"
end
```

Details on the conversion utility program are contained in *MAVRIC Appendix B: MAVRIC Utilities* of the MAVRIC manual.

In SCALE 6.1, the fission source distribution mesh tally produced by KENO contained data representing the number of fissions in each mesh cell in each energy group. In SCALE 6.2, the data stored was changed to be the fissions per

unit volume – the fission density. This is more consistent with other mesh tallies from Monaco which store flux or dose rates that represent averages over the mesh cells. This change also allows the Mesh File Viewer to display the KENO fission source distribution better. The mt2msm utility program also changed from SCALE 6.1 to SCALE 6.2 to account for the change in what is stored in the Keno mesh tally file. Therefore, **KENO-produced fission source mesh tallies and the mt2msm utility should not be mixed-and-matched across versions of SCALE**. Doing so would result in the final Monaco mesh source file being improperly normalized, which would not represent the KENO fission source distribution and would give incorrect results in subsequent MAVRIC calculations. Because there is not a specific 'version flag' in a mesh tally file or mesh source map file, the user must ensure that they have used the same version of SCALE for both the CSAS6 and MAVRIC sequences any time the CAAS capability is used.

2.3.3 MAVRIC input

The input for the MAVRIC portion of the CAAS problem should include the materials and geometry of the criticality model, use the fission distribution as a source, set the source strength, and set any optional modifiers to the source to change its location or add fission photons. The cross section library used by the MAVRIC calculation does not need to have the same group structure as the fission distribution. MAVRIC will automatically convert the fission source group structure to match the group structure of its cross section library.

The shielding calculation needs to specify that the source is the fission distribution file, which is typically "fissionSource.msm". The total source strength can be specified by either the number of fissions in the criticality accident (fission rate or total number) or by the number of released neutrons (the fission rate multiplied by $\bar{v}$ per fission). The value of $\bar{v}$ will be read from the file "kenoNuBar.txt" in the SCALE temporary directory if it is not given in the source input with the keyword "nu-bar=". The mesh source can also be placed at different coordinates in the geometry using the "origin x=*x* y=*y* z=*z*" keywords, if a different reference frame was used with the criticality geometry model that created the mesh source. Rotations of mesh sources are not available at this time. It is also recommended to use filters in the source block to define the source, such as the 'mixture=' filter to only allow source sampling from a specific mixture since the mesh source can be transformed from it's original origin or meshes can cover non-fissionable materials.

For example, using a KENO-VI fission distribution, placing it somewhere in the MAVRIC model and setting the source strength (in neutrons/s) to correspond to 10^{17} fission/s would look like

```
=shell

c
o
p
y
"
C
:
\
m
y
d
o
c
u
~1
\
c
a
a
s
E
x
```

(continues on next page)

```
a
m
p
l
e
\
k
```

(continued from previous page)

```
end

=mavric

...
read
 sources

s
r
c 1

m
e
s
h
S
o
u
r
c
e
F
i
l
e
"
C
:
\
m
y
d
o
c
u
~1
\
c
a
a
s
E
x
a
m
p
l
e
\
f
i
s
s
i
o
n
S
o
u
r
c
e
.
```

(continues on next page)

(continued from previous page)

```
o
r
i
g
i
n
x
=600
y
=650
z
=400

f
i
s
s
i
o
n
s=1.0e17
    end
 src
end
 sources

...
end
 data
end
```

The source strength in neutrons/s will be calculated by MAVRIC to be the fission rate multiplied by the value of read from the "kenoNuBar.txt" file. The neutron strength could have alternatively been specified using the standard source strength keyword "strength=2.5e17" (for an example with the average number of neutrons per fission of 2.5).

The Monte Carlo functional module used by MAVRIC, Monaco, is a fixed-source code. Unless told otherwise, neutrons will multiply in fissionable materials. Since all of the neutrons were part of the source, neutron multiplication should not be allowed and MAVRIC should be run with the keyword "fissionMult=0" in the parameters block. For systems at or near critical without the "fissionMult=0" keyword, Monaco simulations may not end since neutrons will be added to the particle bank at the same rate they leave the system or get killed.

The shielding calculation can be run using standard variance reduction methods (such as path length stretching, user-defined weight windows based on geometry regions, and user-defined source biasing) or using the automated tools which employ approximate discrete-ordinates calculations to determine the space/energy weight windows as well as a biased source distribution in space and energy. The automated tools can be used to optimize the shielding calculation to determine one specific tally using CADIS or several separate tallies or a mesh tally over a large volume of the problem space using FW-CADIS. When using these advanced variance reduction methods, remember to include planes in the discrete-ordinates mesh definition that correspond to the planes in the fission distribution that the source is based on. If they are not included, MAVRIC will resample the fission source on the discrete-ordinates mesh it is using for the importance map, possibly smearing or reducing the original resolution of the fission distribution.

2.4 Example problem

Consider the Jezebel critical plutonium sphere experiment, shown in Fig. 2.1, taking place inside a simple fictitious building, shown in Fig. 2.2. The building has two rooms: an experiment room and a control room. In the control room there is a criticality alarm detector, and it is positioned furthest from the entry to the experiment room. For this example, assume that a criticality excursion results in a total of 10^{18} fissions. This example will calculate the neutron and photon doses seen by a detector in the control room, as well as calculate a dose map for the entire building.

Fig. 2.1: Cutaway view of Jezebel.

2.4.1 KENO-VI criticality and fission source distribution

For the criticality calculation, consider just a bare sphere of plutonium, with a radius of 6.38493 cm. Atom densities (atoms/b·cm) for the sphere material are ^{239}Pu 0.037047; ^{240}Pu 0.0017512; ^{241}Pu 0.00011674; and Cu 0.0013752. This can be easily modeled as a sphere at the origin. For collecting the fission distribution, a uniform mesh grid can be constructed around the sphere, extending 7 cm in each direction, with a 1×1×1 cm voxel size. The first portion of the input files `mavric.caasA.inp` and `mavric.caasB.inp` looks like the following:

```
=csas6

D
o
s
e
R
a
t
e
s
f
r
o
m
a
J
e
```

(continues on next page)

Fig. 2.2: Simple two-room building.

(continued from previous page)

```
v7
-238
n
'-----------------------------------------------------------------------------
' Composition Block
'-----------------------------------------------------------------------------
read
 composition

P
u
-239 1 0 0
.037047   end

P
u
-240 1 0 0
.0017512  end

P
u
-241 1 0 0
.00011674 end

C
u     1 0 0
.0013752  end
end
 composition

'-----------------------------------------------------------------------------
' Parameters Block
'-----------------------------------------------------------------------------
read
 parameters
```

(continues on next page)

(continued from previous page)

```
g
e
n
=250
n
p
g
=200000
n
s
k
=50
h
t
m
=
n
o

c
d
s
=
y
e
s
end
 parameters
'------------------------------------------------------------------------------
' Geometry Block - SCALE standard geometry package (SGGP)
'------------------------------------------------------------------------------
read
 geometry

g
l
o
b
a
l
u
n
i
t 2

s
p
h
e
r
e 1  6
.38493

m
e
d
i
a 1 1 1
v
o
l
=1090
.3277
```

(continues on next page)

(continued from previous page)

```
b
o
u
n
d
a
r
y 1
end
 geometry

'-----------------------------------------------------------------------------
' Grid Block
'-----------------------------------------------------------------------------
read
 gridGeometry

1

t
i
t
l
e
="Mesh for Collecting Fission Distribution"

x
L
i
n
e
a
r 14
-7
.0 7
.0

y
L
i
n
e
a
r 14
-7
.0 7
.0

z
L
i
n
e
a
r 14
-7
.0 7
.0
```

(continues on next page)

(continued from previous page)

```
end
 gridGeometry

end
 data
end

=mt2msm
'fissionSource.3dmap'
1

-1
1

m
a
v
r
i
c
.
c
a
a
s
[
A
/
B
]
.
f
i
s
s
i
o
n
S
o
u
r
c
e
.
m
s
m
'
end
```

The results of this 26 minute calculation are shown in Table 2.1, and details about the calculated fission distribution are shown in Fig. 2.3 and Fig. 2.4.

Table 2.1: Results of the CSAS6 calculation

Quantity	Value	Uncertainty	
k_{eff}	best estimate system k-eff	1.00024	0.00014
$\bar{v}$	system nu bar	3.15671	4.77938E-05

Fig. 2.3: Fission source spatial distribution for the center horizontal slice.

Fig. 2.4: Fission source energy distribution for the center voxel.

2.4.2 MAVRIC transport calculations

Two MAVRIC calculations will be done—one that calculates the doses seen at the detector and one that computes mesh tallies of doses over the entire building. They will share the same materials, geometry, and source but will have different tally and variance reduction options.

The two-room building will be a simple model using concrete-block walls, a concrete floor, and a steel roof, with dimensions shown in Fig. 2.5. The building exterior dimensions are 1200 cm long, 600 cm wide, and 300 cm high above the ground. The exterior and interior walls are all made of a double layer of typical concrete blocks (total of 40 cm thick.) Concrete blocks are typically 39×19×19 cm and weigh ~13.5 kg, since they have a volume fraction of 33.2%. The floor is made of poured concrete, extending 60 cm into the ground. The roof and the exterior door (120 cm wide and 210 cm tall) are made of 1/8 in. (0.3175 cm) thick steel. The experiment room on the left connects to the control room on the right through a maze that prevents radiation streaming. Assume that the critical experiment was in the center of the experiment room, 100 cm above the floor. Assume the detector in the control room is a 30 cm diameter sphere located at position (1145, 55, 285).

Fig. 2.5: Coordinates of the floor, walls, ceiling, and door of the simple block building model (in cm).

If the MAVRIC transport calculation is not in the same file as the CSAS6 calculation, the MAVRIC input would start by moving the KENO-VI results into the SCALE temporary area:

```
=shell

c
o
p
y
%
R
T
N
D
I
R
%
\
c
a
a
s
```

(continues on next page)

```
k
e
n
o
```

(continued from previous page)

```
c
o
p
y
%
R
T
N
D
I
R
%
\
c
a
a
s
.
k
e
n
o
v
i
.
k
e
n
o
N
u
B
a
r
.
t
x
t
k
e
n
o
N
u
B
a
r
.
t
x
t
end
```

The materials and geometry blocks of the two MAVRIC input files for each of the two calculations, `smplprbs/caas.mavricA.inp` and `smplprbs/caas.mavricB.inp`, look like the following:

```
'------------------------------------------------------------------------------
' Composition Block
'------------------------------------------------------------------------------
read
 composition

p
u
-239 1 0 0
.037047   end

p
u
-240 1 0 0
.0017512  end

p
u
-241 1 0 0
.00011674 end

c
u     1 0 0
.0013752  end

o
r
c
o
n
c
r
e
t
e 2 1
.0     293
.0 end

o
r
c
o
n
c
r
e
t
e 3 0
.33198 293
.0 end

s
s304      4 1
.0     293
.0 end
end
 composition
```

(continues on next page)

(continued from previous page)

```
'-------------------------------------------------------------------------------
' Geometry Block - SCALE standard geometry package (SGGP)
'-------------------------------------------------------------------------------
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

c
o
m
="jezebel"

s
p
h
e
r
e   1  6
.38493
o
r
i
g
i
n
x
=280
y
=300
z
=100


c
o
m
="exterior of the building, roof, floor"

c
u
b
o
i
d   10 1200 0    600 0     300
.3175
-60
.0
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d   11 1200 0    600 0     300
.3175 300
.0

c
u
b
o
i
d   12 1200 0    600 0     0
.0
-60


c
o
m
="air space in building - two rooms and maze"

c
u
b
o
i
d   20 1160 40   560 40    300 0


c
o
m
="interior walls to form maze to prevent streaming"

c
u
b
o
i
d   21  560 520  560 120   300 0

c
u
b
o
i
d   22  680 640  480  40   300 0


c
o
m
="exterior door"
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d   30 1200 1160       360 240   210 0

c
u
b
o
i
d   31 1200 1199
.6825  360 240   210 0


c
o
m
="detector sphere"

s
p
h
e
r
e  40   15
.0
o
r
i
g
i
n
x
=1145
y
=55
z
=285


c
o
m
="jezebel"

m
e
d
i
a  1 1   1
v
o
l
=1090
.3277
```

(continues on next page)

(continued from previous page)

```
c
o
m
="walls, roof, floor"

m
e
d
i
a  3 1   10
-20
-11
-12
-30

m
e
d
i
a  4 1   11

m
e
d
i
a  2 1   12


c
o
m
="air space (void) and maze walls"

m
e
d
i
a  0 1   20
-21
-22
-40
-11
-12
-1

m
e
d
i
a  3 1   21
-11
-12

m
e
d
i
a  3 1   22
-11
-12
```

(continues on next page)

(continued from previous page)

```
c
o
m
="exterior door"

m
e
d
i
a  0 1   30
-31

m
e
d
i
a  4 1   31


c
o
m
="detector"

m
e
d
i
a  0 1   40
v
o
l
=14137
.167


b
o
u
n
d
a
r
y 10
end
 geometry
```

The response functions used to compute the doses will be the standard flux-to-dose rate conversion factors for neutrons and photons. These are defined in the definitions block. Note that these responses have units of (rem/hr)/(/cm ^{2}/s).

```
'-----------------------------------------------------------------------------
' Definitions Block
'-----------------------------------------------------------------------------
read
 definitions
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e 5

t
i
t
l
e
="ANSI (1977) neutron flux-to-dose-rate"

s
p
e
c
i
a
l
D
o
s
e
=9029
    end
 response

r
e
s
p
o
n
s
e 6

t
i
t
l
e
="ANSI (1977) photon flux-to-dose-rate"

s
p
e
c
i
a
l
D
o
s
e
=9504
```

(continues on next page)

(continued from previous page)

```
    end
 response
end
 definitions
```

The source used by each MAVRIC simulation will be based on the fission distribution mesh source determined by KENO-VI. The strength of the source can be specified by the total number of fissions that occurred in the criticality event. Fission photons will be added for ^{239}Pu. MAVRIC will determine the total source strength, including the fission photons, from the value of saved by KENO-VI and the multiplicity data from the fission photon data file.

```
'-------------------------------------------------------------------------------
' Sources Block
'-------------------------------------------------------------------------------
read
 sources

s
r
c 1

m
e
s
h
S
o
u
r
c
e
F
i
l
e
=
"
f
i
s
s
i
o
n
S
o
u
r
c
e
.
m
s
m
"

o
r
i
g
i
n
x
=280
y
```

(continues on next page)

(continued from previous page)

```
f
i
s
s
i
o
n
s=1.0e18

m
i
x
t
u
r
e
=1
    end
 src
end
 sources
```

Note that further multiplication needs to be turned off in MAVRIC using the "fissionMult=0" keyword in the parameter block as shown below.

For the responses from the tallies, MAVRIC usually calculates dose rates (rem/hr) using a source strength in particles/s. For this example problem, instead of a source rate, we used a total number of particles (by specifying the number of fissions). Hence, the computed fluxes will have units of particles/cm^2 and the computed responses using the standard dose responses from the cross section libraries will have units of rem s/hr. To get a dose in rem, the responses need to be multiplied by (3600 s/hr)$^{-1}$. This can be done using the MAVRIC tally multiplier keyword.

Each MAVRIC simulation will need a discrete-ordinates mesh. The planes in each dimension where there are material changes are listed in Table 2.2. In addition to these planes, the discrete-ordinates mesh should also subdivide the thick shields in the direction of particle travel. For example, the walls of the maze should be divided to better model the radiation attenuation through the walls in the Denovo calculation. The interior walls of the building will reflect particles, so the first few centimeters are the most important to capture in the importance map. Mesh planes should also be added that correspond to the mesh source after it is placed into the geometry model.

Table 2.2: Main planes in the building

x	y	z
0	0	-60
40	40	0
520	120	210
560	240	300
640	360	300.318
680	480	
1160	560	
1199.68	600	
1200		

Detector doses using CADIS

The grid geometry for this calculation should also include planes that bound the adjoint source, which is the detector area (these values are shown in brackets [] below). The definitions block in `smplprbs/caas.mavricA.inp` also includes the location of the center of the detector, which is used in the adjoint source description.

```
l
o
c
a
t
i
o
n 1

p
o
s
i
t
i
o
n 1145 55 285
 end
 location


g
r
i
d
G
e
o
m
e
t
r
y 1

t
i
t
l
e
="mesh for discrete ordinates 57 x 47 x 31 = 83049"

x
p
l
a
n
e
s 0     10 20 30 35
             40    120 160 240
                   270 272 274 276 278 280 282 284 286 288 290
                   360 440
```

(continues on next page)

(continued from previous page)

```
              520   525 530 550 555
              560   600
              640   645 650 670 675
              680   760 840 920 1000 1080

[1130 1140 1150
]
              1160  1165 1170 1180 1190
              1199
.6825
              1200  end

y
p
l
a
n
e
s 0     10 20 30 35
              40
[50 60
] 70
              120   125 130 140 200
              240   280 290 292 294 296 298 300 302 304 306 308 310
                    320
              360   440 460 470 475
              480
              560   565 570 580 590
              600   end

z
p
l
a
n
e
s
-60
-30
-20
-10
-5
              0     45
                    90 92 94 96 98 100 102 104 106 108 110
                    140 175
              210   255
[280 290
]
              300
              300
.3175   end
 end
 gridGeometry
```

The tallies are region tallies over the detector region (the 10th media card in unit 1) using the appropriate response function for the particle type of the tally. The volume of the detector sphere needs to be listed in the geometry block so that the fluxes and tallies will be correctly computed. The importance map uses standard CADIS to bias the particles

towards the detectors, optimizing the calculation of the total dose (by listing both response functions together, the total response will be used in the adjoint source).

```
'-------------------------------------------------------------------------------
' Tallies Block
'-------------------------------------------------------------------------------
read
 tallies

r
e
g
i
o
n
T
a
l
l
y 1

t
i
t
l
e
="Doses seen by the detector"

n
e
u
t
r
o
n

u
n
i
t
=1
r
e
g
i
o
n
=10

r
e
s
p
o
n
s
e
I
D
=5
```

(continues on next page)

(continued from previous page)

```
m
u
l
t
i
p
l
i
e
r=2.777778e-4
    end
 regionTally

r
e
g
i
o
n
T
a
l
l
y 2

t
i
t
l
e
="Doses seen by the detector"

p
h
o
t
o
n

u
n
i
t
=1
r
e
g
i
o
n
=10

r
e
s
p
o
n
s
e
I
D
=6
```

(continues on next page)

(continued from previous page)

```
m
u
l
t
i
p
l
i
e
r=2.777778e-4
    end
 regionTally
end
 tallies

'------------------------------------------------------------------------------
' Parameters Block - 3 min batch
'------------------------------------------------------------------------------
read
 parameters

r
a
n
d
o
m
S
e
e
d
=3263827

p
e
r
B
a
t
c
h
=654000
b
a
t
c
h
e
s
=40

f
i
s
s
i
o
n
M
u
l
t
=0
```

(continues on next page)

(continued from previous page)

```
end
 parameters

'------------------------------------------------------------------------------
' Importance Map Block
'------------------------------------------------------------------------------
read
 importanceMap

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=1

a
d
j
o
i
n
t
S
o
u
r
c
e 1

l
o
c
a
t
i
o
n
I
D
=1

r
e
s
p
o
n
s
e
I
D
s 5 6 end
```

(continues on next page)

(continued from previous page)

```
    end
 adjointSource
end
 importanceMap
```

The results of this example problem are shown in Table 2.3. Calculation times were 12 minutes for Denovo and 135 minutes for Monaco. Note that the uncertainty for the photon dose is much higher than the neutron dose uncertainty. This is because the simulation was optimized for the calculation of total dose, and the photon component of the total dose is less than 2%. Had a separate calculation been done that used an adjoint source of just the photon response, the photon dose rate uncertainty would have been much smaller but at the expense of the neutron dose rate uncertainty. A single calculation could have also been performed using two adjoint sources, one using the neutron dose response and one using the photon dose response, and forward weighting to help calculate each component of dose with more uniform relative uncertainties.

Table 2.3: Doses seen by the detector

** **	Value	Rel.
Dose	**(rem)**	**Unc.**
neutron	1539	0.78%
photon	30.0	8.00%

Dose map using FW-CADIS

The grid geometry for this calculation does not need extra planes around the detector. The grid geometry in `smplprbs/caas.mavricB.inp` looks like the following:

```
g
r
i
d
G
e
o
m
e
t
r
y 1

t
i
t
l
e
="mesh for discrete ordinates 46x36x23 = 38088"

x
p
l
a
n
e
s 0     10 20 30 35
```

(continues on next page)

(continued from previous page)

```
                40    120 160 240
                      270 272 274 276 278 280 282 284 286 288 290
                      360 440
                520   525 530 550 555
                560   600
                640   645 650 670 675
                680   760 840 920 1000 1080
                1160  1165 1170 1180 1190
                1199
.6825
                1200  end

y
p
l
a
n
e
s 0     10 20 30 35
                40
                120   125 130 140 200
                240   280 290 292 294 296 298 300 302 304 306 308 310
                      320
                360   440 460 470 475
                480
                560   565 570 580 590
                600   end

z
p
l
a
n
e
s
-60
-30
-20
-10
-5
                0     45
                      90 92 94 96 98 100 102 104 106 108 110
                      140 175
                210   255
                300   300
.3175   end
end
 gridGeometry
```

A second grid geometry also needs to be added to the definitions block for the mesh tally to use.

```
g
r
i
d
G
e
o
m
e
t
r
y 2
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="mesh for uniform mesh tally - 40x40x30 cm voxels"

x
L
i
n
e
a
r 30 0
.0 1200
.0

y
L
i
n
e
a
r 15 0
.0  600
.0

z
L
i
n
e
a
r 10 0
.0  300
.0
end
 gridGeometry
```

The mesh tallies for each particle type are listed, along with the appropriate response function. The importance map uses FW-CADIS to better spread the particles out over the entire geometry, optimized for the calculation of total dose in the void regions.

```
'------------------------------------------------------------------------------
' Tallies Block
'------------------------------------------------------------------------------
read
 tallies

m
e
s
h
T
a
l
```

(continues on next page)

```
l
y 1
```

(continued from previous page)

```
t
i
t
l
e
="Neutron doses mapped over the entire building"

n
e
u
t
r
o
n

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=2

r
e
s
p
o
n
s
e
I
D
=5

n
o
G
r
o
u
p
F
l
u
x
e
s
```

(continues on next page)

(continued from previous page)

```
m
u
l
t
i
p
l
i
e
r=2.777778e-4
    end
 meshTally

m
e
s
h
T
a
l
l
y 2

t
i
t
l
e
="Photon doses mapped over the entire building"

p
h
o
t
o
n

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=2

r
e
s
```

(continues on next page)

```
p
o
n
s
e
I
D
```

(continued from previous page)

```
n
o
G
r
o
u
p
F
l
u
x
e
s

m
u
l
t
i
p
l
i
e
r=2.777778e-4
    end
 meshTally
end
 tallies

'-------------------------------------------------------------------------------
' Parameters Block - 3 min batch
'-------------------------------------------------------------------------------
read
 parameters

r
a
n
d
o
m
S
e
e
d
=3263827

p
e
r
B
a
t
c
h
=669000
b
a
t
c
h
e
s
```

(continues on next page)

(continued from previous page)

```
f
i
s
s
i
o
n
M
u
l
t
=0
end
 parameters

'------------------------------------------------------------------------------
' Importance Map Block
'------------------------------------------------------------------------------
read
 importanceMap

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=1

a
d
j
o
i
n
t
S
o
u
r
c
e 1

b
o
u
n
d
i
n
g
B
o
x 1200 0  600 0  300
.3175
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e
I
D
s 5 6 end

m
i
x
t
u
r
e
=0
    end
 adjointSource

r
e
s
p
W
e
i
g
h
t
i
n
g
end
 importanceMap
```

This calculation used 5 minutes for the forward Denovo S_N calculation, 6 minutes for the adjoint Denovo, and 120 minutes for the Monaco Monte Carlo. The resulting mesh tally is shown in Fig. 2.6. The uncertainties for each voxel are shown in Fig. 2.7. Note that the dose in the voxel containing the detector (not shown in the figures) is 1.552×10^3 rem with a relative uncertainty of 3.8%, closely matching the value calculated with the first MAVRIC simulation.

Similar to the detector doses above, a single calculation could have also been performed for the dose maps using two adjoint sources, one using the neutron dose response and one using the photon dose response, and forward weighting to help calculate each component of dose with more uniform relative uncertainties.

Fig. 2.6: Dose (rem) results for the z=100 cm plane (containing the source).

Fig. 2.7: Relative uncertainties in the dose, most less than 1%, for the z=100 cm plane.

2.5 Summary

SCALE now has the capability to do detailed simulations of criticality accident alarm systems. The advanced variance reduction capabilities of the MAVRIC radiation transport sequence allow for the full three-dimensional analysis of CAAS problems in reasonable amounts of computer time. This enables the use of more realistic source definitions, such as a detailed spatial/energy dependent fission source distribution determined by the KENO-VI criticality code, and the critical assembly itself can be included in the transport model.

CHAPTER

THREE

MAVRIC APPENDIX B: MAVRIC UTILITIES

3.1 Introduction

Several utilities are provided to aid users in dealing with some of the output files produced by Monaco and MAVRIC. These utilities were developed at ORNL for specific projects and have been added to SCALE so that all users can benefit. More utilities have been added that deal with Denovo, including the older *.varscl files for flux output used in SCALE 6.1 and the current binary *.dff file for flux output used in SCALE 6.2. These tools do not have the modern block/keyword input structure but instead have a fixed format, which is fairly simple since each utility is made for a very specific function.

Each is described in the following sections. Five sample problems, `mavricUtilities1.inp`, ``mavricUtilities2.inp`, `mavricUtilities3.inp`, `mavricUtilities4.inp` and `mavricUtilities5.inp` demonstrate the use of some of these. For all of these utilities, filenames should be enclosed in quotes.

3.2 Utilities working with Monaco mesh tally (*.3DMAP) files

mt2ascii	Convert a mesh tally into an ASCII text file.
mt2msl	Convert a mesh tally into a mesh source lite.
mt2msm mt2silo	Convert a mesh tally into a mesh source. Convert a mesh tally file into a Silo file for VisIt.
mt2vtk	Convert one dataset of one family in a mesh tally to VTK format.
mtAdder	Add several Monaco mesh tally files together into one mesh tally.
mtAverager	Average several Monaco mesh tally files into one mesh tally.
mtBinOp	Binary operation of mesh tally files: sum, difference, product, and ratio.
mtDisp	Display the basics of a mesh tally file.
mtExpand	Expand a space-only mesh from a mesh tally with an energy function.
mtFilter	Perform various filters on a mesh tally file.
mtInv	Invert all of the values in a mesh tally.
mtMask	Keep only or remove specified voxels of a mesh tally based on geometry.
mtMinMax	Find the location/value of the min or max of each real mesh in a mesh tally.
mtMultiply	Multiply a mesh tally by a constant factor.
mtPull	Pull values from certain voxels out of a mesh tally file.
mtRefine	Subdivide the mesh into smaller meshes for better visualization.
mtResp	Apply a response function to one family of a mesh tally file.
mtSplit	Split off part of a mesh tally file into a separate mesh tally file.

mt2ascii - Convert a mesh tally into an ASCII text file.

Intended use: Since mesh tally files are in binary, the viewer can be used to list mesh values. To get the values from the entire file, this utility can be used to create an ASCII text version.

Input: The mesh tally file name and the filename for the resulting ASCII file

Output: An ASCII formatted file

Example:

```
=mt2ascii

"
/
o
p
t
i
o
n
a
l
/
p
a
t
h
/
m
e
s
h
T
a
l
l
y
F
i
l
e
n
a
m
e
.3
d
m
a
p
"
!
t
h
e
m
e
s
h
t
a
l
l
```

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(continued from previous page)

```
"
/
o
p
t
i
o
n
a
l
/
p
a
t
h
/
o
u
t
p
u
t
F
i
l
e
n
a
m
e
.
t
x
t
"
!
o
u
t
p
u
t
f
i
l
e
n
a
m
e
end
```

mt2msl - Convert a mesh tally into a mesh source lite.

Intended use: Convert a fissionSource.3dmap mesh tally computed by KENO into a meshSoureLite (*.msl) file that can be used by a subsequent KENO run using starting source type nst=9.

Input: Name of mesh tally (*.3dmap) file

Output: A mesh source lite (*.msl) file

Example:

```
=mt2msl
"input.3dmap"
!
m
e
s
h
f
i
l
e
(
*
.3
d
m
a
p
)
n
a
m
e
1
!
f
a
m
i
l
y
14
!
g
r
o
u
p
,
o
r 0
f
o
r
f
a
m
i
l
y
t
o
t
a
l
```

(continues on next page)

(continued from previous page)

```
"result.msl"
!
m
e
s
h
s
o
u
r
c
e
l
i
t
e
(
*
.
m
s
l
)
f
i
l
e
n
a
m
e
end
```

mt2msm - Convert a mesh tally into a mesh source.

Intended use: Turn a tally of fission rate data into a mesh source file. Mesh tallies are stored in a generic *.3dmap format, which consist of several families, each with one or more datasets. A typical mesh tally (without the "noGroupFluxes" keyword) contains three families: the neutron fluxes with each energy group as a dataset, the photon fluxes with each energy group as a data set, and the responses with each response as a dataset. This program uses the spatial information of the mesh tally and combines a user-given energy distribution for all voxels. A second way to use this program is to use a whole family (all the energy groups) without a user-given energy distribution.

Input:

Line 1: filename of mesh tally

Line 2: which family of tally

Line 3: which dataset of that family (or 0 for sum of family)

Line 4: source type: 1-neutron, 2-photon

Line 5: number of bins for mesh source

Lines : energy (eV) and pdf values

Lines : energy (eV) and pdf values

... ...

Lines : energy (eV) and pdf values

Line : energy (eV)

Line last: desired output name

Input:

Line 1: filename of mesh tally

Line 2: which family of tally

Line 3: -1 (meaning use the whole family)

Line 4: source type: 1-neutron, 2-photon

Line 5: desired output name

Output: The resulting mesh source stored with the desired filename

Notes: Statistics of mesh tally are discarded.

Example:

```
=shell

c
p
$
{
R
T
N
D
I
R
}
/
b
a
r
r
e
l1
.
m
t1
.3
d
m
a
p
.
end

=mt2msm

"
b
a
r
r
e
l1
```

(continues on next page)

```
.
m
t1
.3
d
m
a
```

(continued from previous page)

```
3
!
m
e
s
h
t
a
l
l
y
f
a
m
i
l
y
(1
-
n
, 2
-
p
, 3
-
r
e
s
p
o
n
s
e
s
)
1
!
r
e
a
l
m
e
s
h
i
n
t
h
a
t
f
a
m
i
l
y
```

(continues on next page)

```
(0
m
e
a
n
s
t
```

(continued from previous page)

```
1
!
m
e
s
h
s
o
u
r
c
e
p
a
r
t
i
c
l
e
t
y
p
e   1
-
n
e
u
t
r
o
n
, 2
-
p
h
o
t
o
n
143
!
n
u
m
b
e
r
o
f
b
i
n
s
i
n
b
i
n
n
e
d
h
i
```

(continues on next page)

(continued from previous page)

```
1
.9640
E
+07 1
.29403
E
-08
!
E
_1
p
d
f
_1
1
.7332
E
+07 4
.60970
E
-07
!
E
_2
p
d
f
_2
1
.6905
E
+07 2
.56619
E
-06
!
E
_3
p
d
f
_3

.
.
.
.
.
.
1
.2341
E
+03 5
.28408
E
-06
!
E
_142
p
d
f
_142
```

(continues on next page)

(continued from previous page)

```
9
.6112
E
+02 1
.77756
E
-06
!
E
_143
p
d
f
_143
7
.4852
E
+02
!
E
_144

"
b
a
r
r
e
l
.
f
i
s
s
i
o
n
.
m
s
m
"
!
o
u
t
p
u
t
f
i
l
e
n
a
m
e
```

(continues on next page)

(continued from previous page)

```
end

=shell

c
p
b
a
r
r
e
l
.
f
i
s
s
i
o
n
.
m
s
m
$
{
R
T
N
D
I
R
}
end
```

Example:

```
=mt2msm

"
f
i
s
s
i
o
n
S
o
u
r
c
e
.3
d
m
a
p
"
```

(continues on next page)

(continued from previous page)

```
1
!
n
e
u
t
r
o
n
f
l
u
x
(
f
o
r
K
E
N
O 3
d
m
a
p
f
i
l
e
s
t
h
e
r
e
i
s
o
n
l
y
o
n
e
f
a
m
i
l
y
)

-1
!
u
s
e
t
h
e
w
h
o
l
```

(continues on next page)

(continued from previous page)

```
1
!
p
a
r
t
i
c
l
e
t
y
p
e
(
n
e
u
t
r
o
n
)

"
c
a
a
s
.
k
e
n
o
v
i
.
f
i
s
s
i
o
n
S
o
u
r
c
e
.
m
s
m
"
end
```

In SCALE 6.1, the fission source distribution mesh tally produced by KENO contained data representing the number of fissions in each mesh cell in each energy group. In SCALE 6.2, the data stored was changed to be the fissions per unit volume – the fission density. This is more consistent with other mesh tallies from Monaco which store flux or dose rates that represent averages over the mesh cells. This change also allows the MeshFileViewer to display the KENO fission source distribution better. The mt2msm utility program also changed from SCALE 6.1 to SCALE 6.2 to account for the change in what is stored in the KENO mesh tally file. Therefore, **KENO-produced fission source mesh tallies and the mt2msm utility should not be mixed-and-matched across versions of SCALE.** Doing so would result in the final Monaco mesh source file being improperly normalized, which would not properly represent the KENO fission source distribution and would give incorrect results in subsequent MAVRIC calculations. Because there is not a specific 'version flag' in a mesh tally file or mesh source map file, the user must ensure that they have used the same version of SCALE for both the CSAS6 and MAVRIC sequences any time the CAAS capability is used.

mt2silo - Convert a mesh tally file into a Silo file for VisIt.

Input: Name of mesh file (*.3dmap), name of a Silo file, and a format

Output: A new Silo file

Notes: For format, use either 2 (PDB) or 7 (HDF5).

Example:

```
=mt2silo
"perfect.3dmap"
!
t
h
e
e
x
i
s
t
i
n
g
m
e
s
h
t
a
l
l
y
"perfect.silo"
!
t
h
e
n
e
w
s
i
l
o
f
i
l
e
```

(continues on next page)

(continued from previous page)

```
7
!
f
o
r
m
a
t
-
H
D
F5
end
```

mt2vtk - Convert one dataset of one family in a mesh tally to VTK format.

Intended use: This is a way to transfer Monaco mesh tally data into a common format that can be used by many data visualization packages, including VisIt. Mesh tallies are stored in a generic *.3dmap format, which consist of several families, each with one or more datasets. A typical mesh tally contains three families: the neutron fluxes with each energy group as a dataset, the photon fluxes with each energy group as a data set, and the responses with each response as a dataset. This program selects one dataset of one family and saves the data (and optionally the absolute uncertainties) in an ASCII file using a VTK file format.

Input: The mesh file name, which family, which dataset of that family, whether or not to include absolute uncertainties and the filename for the resulting VTK file

Output: An ASCII VTK-formatted file

Example:

```
=mt2vtk

"
/
o
p
t
i
o
n
a
l
/
p
a
t
h
/
m
e
s
h
T
a
l
l
y
F
```

(continues on next page)

```
i
l
e
n
a
m
e
```

(continued from previous page)

```
1
!
n
e
u
t
r
o
n
f
l
u
x
f
a
m
i
l
y
5
!
e
n
e
r
g
y
g
r
o
u
p 5

t
r
u
e
!
i
n
c
l
u
d
e
u
n
c
e
r
t
a
i
n
t
i
e
s
```

(continues on next page)

(continued from previous page)

```
"
/
o
p
t
i
o
n
a
l
/
p
a
t
h
/
o
u
t
p
u
t
F
i
l
e
n
a
m
e
.
v
t
k
"
!
o
u
t
p
u
t
f
i
l
e
n
a
m
e
end
```

Example:

```
=mt2vtk
```

(continues on next page)

```
"
/
o
p
t
i
o
```

(continued from previous page)

```
3
!
t
h
e
r
e
s
p
o
n
s
e
f
a
m
i
l
y
1
!
f
i
r
s
t
r
e
s
p
o
n
s
e

f
a
l
s
e
!
d
o
n
o
t
i
n
c
l
u
d
e
u
n
c
e
r
t
a
i
n
t
i
```

(continues on next page)

(continued from previous page)

```
"
/
o
p
t
i
o
n
a
l
/
p
a
t
h
/
o
u
t
p
u
t
F
i
l
e
n
a
m
e
.
v
t
k
"
!
o
u
t
p
u
t
f
i
l
e
n
a
m
e
end
```

mtAdder - Add several Monaco mesh tally files together into one mesh tally.

Intended use: Add mesh tally results from different sources into one tally. The resulting mesh tally is the sum of all the components in the several mesh tallies—fluxes are added and responses are added. For example, two runs of MAVRIC

from two different sources can be made. The mesh tally results can then be added together, getting the total fluxes and total responses from each.

Input: The number of files, followed by the list of mesh tally filenames to add, then the name of the total mesh tally

```
=
m
t
A
d
d
e
r

n

"
f
i
l
e
n
a
m
e
_1
"

"
f
i
l
e
n
a
m
e
_2
"

.
.
.

"
f
i
l
e
n
a
m
e
_
n
"

"
```

(continues on next page)

```
r
e
s
u
l
t
F
```

(continued from previous page)

```
end
```

Output: A new mesh tally file

Notes: All of the mesh tally files must be the same size and shape (number of families, x cells, y cells, z cells, and energy groups in each family) and have the same number of responses. Responses (if any) must be consistent to calculate meaningful results.

Example:

```
=mtAdder
3

"
m
e
s
h
F
i
l
e
n
a
m
e
_1
.3
d
m
a
p
"

"
m
e
s
h
F
i
l
e
n
a
m
e
_2
.3
d
m
a
p
"

"
m
e
s
h
F
i
l
e
n
```

(continues on next page)

(continued from previous page)

```
"
m
e
s
h
F
i
l
e
n
a
m
e
T
o
t
a
l
.3
d
m
a
p
"
end
```

mtAverager - Average several Monaco mesh tally files into one mesh tally.

Intended use: Combine (average) separate runs of the same problem with different random number seeds into one tally. For example, if a user does 10 separate runs of the same problem (poor man's parallel) and wants to combine the results as if they were from one run, an average is needed. The average and uncertainties are weighted by the number of histories in each run, to maintain proper statistics.

Input: The number of files, each filename and how many histories, then the name of the total mesh tally

```
=mtAverager

n

"
f
i
l
e
n
a
m
e
_1
"
h
i
s
t
o
r
i
e
s
5
```

(continues on next page)

(continued from previous page)

```
"
f
i
l
e
n
a
m
e
_2
"
h
i
s
t
o
r
i
e
s
_2

.
.
.
.
.
.

"
f
i
l
e
n
a
m
e
_
n
"
h
i
s
t
o
r
i
e
s
_
n

"
r
e
s
u
l
t
F
i
l
```

(continues on next page)

(continued from previous page)

```
end
```

Output: A new mesh tally file

Notes: All of the mesh tally files must be the same size and shape (number of families, x cells, y cells, z cells, and energy groups in each family) and have the same number of responses. Responses (if any) must be consistent to calculate meaningful results.

Example:

```
=mtAverager
3

"
m
e
s
h
F
i
l
e
n
a
m
e
_1
.3
d
m
a
p
"    800000

"
m
e
s
h
F
i
l
e
n
a
m
e
_2
.3
d
m
a
p
"    900000

"
m
e
```

(continues on next page)

```
s
h
F
i
l
e
n
```

(continued from previous page)

```
"
/
h
o
m
e
/
a
r
e
a
/
m
e
s
h
F
i
l
e
n
a
m
e
.
a
v
e
.3
d
m
a
p
"
end
```

mtBinOp - Binary operation of mesh tally files: sum, difference, product, and ratio.

Intended use: Apply simple math to the results stored in mesh tally files

Input: The first mesh tally, the operator: add (or sum, +), subtract (or difference, -), multiply (or product, x, *) and divide (or ratio, ÷," /"), the second mesh tally name and then name of the resulting mesh tally file.

Output: A new mesh tally file

Notes: Uncertainties are propagated assuming the two mesh tallies are uncorrelated, which may not always be a good assumption. Mesh tallies need to have the same grid structure and number of families and groups. Dataset names in the results are inherited from the first mesh tally and may not make sense after the operation. When using the / (slash) for division, enclose it in quotes ("/").

```
=mtBinOp

"
n
e
u
t
r
o
n
.3
d
m
a
```

(continues on next page)

(continued from previous page)

```
d
i
v
i
d
e
!
o
p
e
r
a
t
i
o
n

"
t
o
t
a
l
.3
d
m
a
p
"
!
s
e
c
o
n
d
o
p
e
r
a
n
d

"
r
a
t
i
o
.3
d
m
a
p
"
!
o
u
t
p
u
t
```

(continues on next page)

(continued from previous page)

```
end
```

mtDisp - Display the basics of a mesh tally file.

Input: A mesh tally (*.3dmap) file

Output: Some of the basic details of mesh file

Example:

```
=mtDisp
"simulation.mt2.dff"
!
e
x
i
s
t
i
n
g
m
e
s
h
f
i
l
e
end
```

mtExpand - Expand a space-only mesh from a mesh tally with an energy function

Input: A mesh tally (*.3dmap) file and some parameters

Output: A mesh file similar to a mesh source but with uncertainty

Example:

```
=mtExpand
'activate.mt1.3dmap'
2 1
!
r
e
s
p
o
n
s
e
f
a
m
i
l
y
,
f
i
r
s
t
r
e
s
p
```

(continues on next page)

(continued from previous page)

```
t
r
u
e
!
m
u
l
t
i
p
l
y
b
y
v
o
x
e
l
v
o
l
u
m
e
s
2
!
m
a
k
e
p
h
o
t
o
n
s
o
u
r
c
e
19
!
g
r
o
u
p
s
2
.00
E
+07 0
```

(continues on next page)

(continued from previous page)

```
1
.00
E
+07 0
8
.00
E
+06 0
6
.50
E
+06 0
5
.00
E
+06 0
4
.00
E
+06 0
3
.00
E
+06 0
2
.50
E
+06 0
2
.00
E
+06 0
1
.66
E
+06 0
.5
1
.33
E
+06 1
.5
1
.00
E
+06 0
8
.00
E
+05 0
6
.00
E
+05 0
4
.00
E
+05 0
```

(continues on next page)

(continued from previous page)

```
3
.00
E
+05 0
2
.00
E
+05 0
1
.00
E
+05 0
4
.50
E
+04 0
1.00E+04
'photonSource.3dmap'
end
```

mtFilter - Perform various filters on a mesh tally file.

Input: A *.3dmap mesh tally file and a group-wise response function

Output: A *.3dmap mesh tally file

Notes: Three basics types of filters: 0) flattening filter, 1) high-pass filter, 2) low-pass filter. For types 1 and 2, the values plus a given number of standard deviations will be compared to the criteria. The input list depends on filter type. Types 1 and 2 require a value and a number of standard deviations (n_sigma). A flattening filter turns any positive value into the value of "1.0".

Filtering performed based on following comparisons;

value + n_sigmas*abs_unc > minValue (high-pass)

or

value + n_sigmas*abs_unc < maxValue (low-pass)

The number of sigmas can be positive or negative.

Examples:

```
=mtFilter
"doseRates.3dmap"
!
e
x
i
s
t
i
n
g
m
e
s
h
t
a
l
l
y
```

(continues on next page)

```
f
i
l
e
```

(continued from previous page)

```
1
!
h
i
g
h
-
p
a
s
s
f
i
l
t
e
r
:
0
.150
!
k
e
e
p
d
o
s
e
r
a
t
e
s
a
b
o
v
e 0
.150

-3
.0
!
a
d
d
-3
.0
s
t
a
n
d
a
r
d
d
e
v
i
a
t
i
```

(continues on next page)

(continued from previous page)

```
"above.3dmap"
!
n
e
w
m
e
s
h
t
a
l
l
y
f
i
l
e
end

=mtFilter
"above.3dmap"
!
e
x
i
s
t
i
n
g
m
e
s
h
t
a
l
l
y
f
i
l
e
0
!
f
l
a
t
t
e
n
i
n
g
f
i
l
t
e
r
```

(continues on next page)

(continued from previous page)

```
"boolean.3dmap"
!
n
e
w
m
e
s
h
t
a
l
l
y
f
i
l
e
end
```

mtInv - Invert all of the values in a mesh tally.

Intended use: Invert non-zero values in a mesh tally to be used in further processing.

Input: The original mesh tally, the name of the resulting mesh tally file

Output: A new mesh tally file

Notes: Uncertainties are propagated (the relative uncertainty of the reciprocal of a value is the same as the relative uncertainty of the value).

Example:

```
=mtInv
'someTally.3dmap'       ! existing mesh tally file
'inverted.3dmap'        ! new mesh tally file
end
```

mtMask - Keep only or remove specified voxels of a mesh tally based on geometry.

Intended use: Only keep or remove certain portions of a mesh tally based on the unit, media, or mixture at the center of the voxel.

Input: A mesh tally file, an action (keeponly or remove), an operation (intersection or union) of the unit=u, media=r and mixture=m, a replacement value for voxels not kept and the file name of the resulting mesh tally file. User can specify things such as 1) keep only the voxels that have unit=2 and mixture=5, 2) keep only the voxels that have media=3 or mixture=4, 3) remove voxels that have unit=2 and mixture=5, 4) remove voxels that have media=3 or mixture=4. To not include the unit, media, or mixture in the specification, use a value of -1.

Output: A new mesh tally file.

Notes: When processing a file before finding the maximum, make the replacement value something very low. If mtMask is being used before finding the minimum, then set the replacement value high. Media is the SGGP media number within the unit.

```
=mtMask
"theTally.3dmap"
!
e
x
```

(continues on next page)

```
i
s
t
i
n
g
m
```

(continued from previous page)

```
k
e
e
p
o
n
l
y
!
u
s
e 'keeponly'
o
r 'remove'

i
n
t
e
r
s
e
c
t
i
o
n
!
u
s
e 'intersection'
o
r 'union'
2
-1 5
!
u
n
i
t
=2
A
N
D
m
i
x
t
u
r
e
=5
0
.0
!
r
e
p
l
a
c
e
m
```

(continues on next page)

(continued from previous page)

```
'new.3dmap'             ! new mesh tally file
end

=mtMask
"theTally.3dmap"
!
e
x
i
s
t
i
n
g
m
e
s
h
t
a
l
l
y
f
i
l
e

r
e
m
o
v
e
!
u
s
e 'keeponly'
o
r 'remove'

u
n
i
o
n
!
u
s
e 'intersection'
o
r 'union'

-1 3 4
!
m
e
d
i
a
-3
O
R
m
```

(continues on next page)

(continued from previous page)

```
0
.0
!
r
e
p
l
a
c
e
m
e
n
t
v
a
l
u
e
f
o
r
v
o
x
e
l
s
r
e
m
o
v
e
d
'new.3dmap'             ! new mesh tally file
end
```

mtMinMax - Find the location/value of the min or max of each real mesh in a mesh tally.

Intended use: Determine the minimum or maximum values in a mesh tally.

Input: The mesh tally, what to find (minimums or maximums), how many mins/maxs for each real mesh in the mesh tally, and the name of the text output file to store the results

Output: A text output containing the values and locations of the minimums or maximums of each real mesh in a tally file

Notes: The same information is also in the main SCALE output file.

Example:

```
=mtMinMax
'bigOleMeshTally.3dmap'   ! existing mesh tally file

m
a
x
i
```

(continues on next page)

```
m
u
m
!
f
i
n
```

(continued from previous page)

```
5
!
l
i
s
t
t
o
p 5
m
a
x
i
m
u
m
v
a
l
u
e
s
i
n
e
a
c
h
r
e
a
l
m
e
s
h
'theList.txt'              ! file name to store all of the results
end
```

mtMultiply - Multiply a mesh tally by a constant factor.

Intended use: Multiply every group of every family in a mesh tally for either a change in source strength or a change in units.

Input: The original mesh tally, the multiplier, and the name of the resulting mesh tally file

Output: A new mesh tally file

Example:

```
=mtMultiply

"
s
i
m
u
l
a
t
i
```

(continues on next page)


```
n
.
m
t1
```

(continued from previous page)

```
25
.0
!
s
o
u
r
c
e
s
t
r
e
n
g
t
h
i
n
c
r
e
a
s
e
o
f 25

"
s
i
m
u
l
a
t
i
o
n
.
b
i
g
g
e
r
.3
d
m
a
p
"
!
o
u
t
p
u
t
f
i
l
e
n
```

(continues on next page)

(continued from previous page)

```
end
```

mtPull - Pull values from certain voxels out of a mesh tally file.

Intended use: Get energy-dependent fluxes for certain locations from a mesh file.

Input: A mesh file (*.3dmap) file and a list of positions and/or voxels

Output: Listing of energy-dependent fluxes from each desired location to an ASCII text file

Notes: Can pull fluxes either by a physical coordinate position or by voxel indices. Positions should be entered as a set of x, y, z for Cartesian coordinate system and r, , z for cylindrical coordinate system.

Example:

```
=mtPull
"duh.mt2.3dmap"
!
e
x
i
s
t
i
n
g
m
e
s
h
f
i
l
e

n
!
n
u
m
b
e
r
o
f
x
,
y
,
z
p
o
i
n
t
s
t
o
p
u
l
l
```

(continues on next page)

(continued from previous page)

```
x
_1
y
_1
z
_1
!
c
o
o
r
d
i
n
a
t
e
s
o
f
p
o
i
n
t 1

x
_1
y
_2
z
_2
!
c
o
o
r
d
i
n
a
t
e
s
o
f
p
o
i
n
t 2

.
.
.
```

(continues on next page)

```
x
_
n
y
_
n
z
```

(continued from previous page)

```
m
!
n
u
m
b
e
r
o
f
i
,
j
,
k
v
o
x
e
l
s
t
o
p
u
l
l

i
_1
j
_1
k
_1
!
i
n
d
i
c
e
s
o
f
v
o
x
e
l 1

i
_2
j
_2
k
_2
!
i
n
d
i
c
e
```

(continues on next page)

(continued from previous page)

```
.
.
.

i
_
m
j
_
m
k
_
m
!
i
n
d
i
c
e
s
o
f
v
o
x
e
l
m
"outputName.txt"
!
n
a
m
e
o
f
o
u
t
p
u
t
t
e
x
t
f
i
l
e
=end
```

mtRefine - Subdivide the mesh into smaller meshes.

Input: A *.3dmap mesh tally file with geometry mesh size (I,J,K) and three integers describing how many subdivisions of each voxel to create in each dimension

Output: A *.3dmap mesh tally file with geometry mesh size (I*nx,J*ny,K*nz)

Example:

```
=mtRefine
"fluxes.3dmap"
!
e
x
i
s
t
i
n
g
*
.3
d
m
a
p
m
e
s
h
t
a
l
l
y
f
i
l
e
(
I
,
J
,
K
)

n
x
n
y
n
z
!
h
o
w
t
o
s
u
b
d
i
v
i
d
e
e
a
c
```

(continues on next page)

(continued from previous page)

```
"refined.3dmap"
!
n
e
w
(
l
a
r
g
e
r
e
r
)
*
.3
d
m
a
p
m
e
s
h
t
a
l
l
y
f
i
l
e
(
I
*
n
x
,
J
*
n
y
,
K
*
n
z
)
end
```

mtResp - Apply a response function to one family of a mesh tally file.

Intended use: Compute group-wise dose or reaction rates by combining a response function with the scalar fluxes.

Input: A *.3dmap mesh tally file and a group-wise response function

Output: A *.3dmap mesh tally file containing one family

Example:

```
=mtResp
"fluxes.3dmap"
!
e
x
i
s
t
i
n
g
*
.3
d
m
a
p
m
e
s
h
t
a
l
l
y
f
i
l
e
200
!
n
u
m
b
e
r
o
f
b
i
n
s
i
n
r
e
s
p
o
n
s
e
```

(continues on next page)

(continued from previous page)

```
1
!
w
h
i
c
h
f
a
m
i
l
y
2
.2675480
E
-04
!
r
e
s
p
o
n
s
e
g
r
o
u
p 1
2
.2283355
E
-04
!
r
e
s
p
o
n
s
e
g
r
o
u
p 2
2
.1878259
E
-04
!
r
e
s
```

(continues on next page)

```
p
o
n
s
e
g
r
```

(continued from previous page)

```
.
.
.
3
.6748440
E
-06
!
r
e
s
p
o
n
s
e
g
r
o
u
p
n
b
i
n
s
-2
3
.6748443
E
-06
!
r
e
s
p
o
n
s
e
g
r
o
u
p
n
b
i
n
s
-1
3
.6748436
E
-06
!
```

(continues on next page)

```
r
e
s
p
o
n
s
```

(continued from previous page)

```
"doseByGroup.3dmap"
!
n
e
w
(
s
m
a
l
l
e
r
)
*
.3
d
m
a
p
m
e
s
h
t
a
l
l
y
f
i
l
e
end
```

mtSplit - Split off part of a mesh tally file into a separate mesh tally file.

Intended use: Some mesh tallies may become so large that the MeshFileViewer cannot load the entire file to view. This utility allows users to split off one family or just one group of one family into a separate mesh tally file.

Input: The original mesh tally, which family (neutron, photon, or responses), and which dataset (usually a group). Instead of a dataset, users may specify 0 to get the total of a family or -1 to get all datasets for that family. The name of the resulting mesh tally also needs to be given.

Output: A new, smaller, mesh tally file

Example:

```
=mtSplit

"
m
a
v
r
i
c
U
t
i
l
```

(continues on next page)


```
t
i
e
s3
```

(continued from previous page)

```
1
!
t
h
e
f
a
m
i
l
y
o
f
n
e
u
t
r
o
n
f
l
u
x
e
s
5
!
f
i
f
t
h
n
e
u
t
r
o
n
f
l
u
x
g
r
o
u
p

"
m
a
v
r
i
c
U
t
i
i
t
i
```

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```
end
```

3.3 Utilities for working with DENOVO binary flux (*.dff) files

These utilities include the following:

dff2dso	Convert a Denovo flux file into a Denovo spatial output file.
dff2mai	Convert a Denovo flux file into a mesh angular information file.
dff2mim	Invert a Denovo flux file and store as a mesh importance map.
dff2msl	Convert a Denovo flux file into a mesh source lite.
dffBinOp	Binary operation of Denovo flux files: sum, difference, product, and ratio.
dffDisp	Display the basics of a Denovo flux file.
dffExpand	Expand a space-only Denovo flux file by an energy function.
dffFilter	Perform various filters on a Denovo flux file.
dffFix	Fix the zero and negative values in a Denovo flux file.
dffInt	Integrate a single particle type from a Denovo flux file.
dffInv	Invert the values in a Denovo flux file.
dffMult	Multiply a Denovo flux file by a constant factor.
dffPull	Pull fluxes from certain voxels out of a Denovo flux file.
dffResp	Apply a response function to scalar fluxes in a Denovo flux file.
dffSplit	Split off a single particle type from a Denovo flux file.

dff2dso - Convert a Denovo flux file into a Denovo spatial output file.

Input: A binary (stream) Denovo flux file and which particle types to convert

Output: A binary (stream) Denovo Spatial Output file

Notes: For particle type, use 1 for neutron, 2 for photon, and 0 for all types.

Example:

```
=dff2dso
"neatStuff.dff"
!
e
x
i
s
t
i
n
g
D
e
n
o
v
o
f
l
u
x
f
i
l
```

(continues on next page)

(continued from previous page)

```
1
!
k
e
e
p
o
n
l
y
n
e
u
t
r
o
n
i
n
f
o
r
m
a
t
i
o
n
"neatStuff.dso"
!
n
e
w
D
e
n
o
v
o
s
p
a
t
i
a
l
o
u
t
p
u
t
f
i
l
e
end
```

dff2mai - Convert a Denovo flux file into a mesh angular information file.

Intended use: Take the optional net current information from a Denovo flux file and create the adjoint current unit vectors and lambda parameters required for directional CADIS. This is stored in a mesh angular information (*.mai) file.

Input: A binary (stream) denovoFluxFile

Output: A binary (stream) meshAngularInfoFile, a mesh angular information file

Example:

```
=dff2mai
"mavricUtilities3.adjoint.dff"
!
n
e
w
d
e
n
o
v
o
F
l
u
x
F
i
l
e
"mavricUtilities3.mai"
!
m
e
s
h
a
n
g
u
l
a
r
i
n
f
o
f
i
l
e
end
```

dff2mim - Invert a Denovo flux file and store as a mesh importance map.

Intended use: Make weight targets without a consistent biased mesh source.

Input: A Denovo flux (*.dff) file, a scalar constant, and the name of Monaco mesh importance map (*.mim) file.

Output: A Monaco mesh importance map (*.mim) file.

Example:

```
=dff2mim
"adjoint.dff"
!
e
x
i
s
t
i
n
g
a
d
j
o
i
n
t
d
e
n
o
v
o
F
l
u
x
F
i
l
e
3
.0
e
-10
!
c
o
n
s
t
a
n
t
t
a
r
g
e
t
W
e
i
g
h
t
=
c
o
n
s
```

(continues on next page)

(continued from previous page)

```
"test.mim"
!
n
e
w
M
o
n
a
c
o
m
e
s
h
i
m
p
o
r
t
a
n
c
e
m
a
p
end
```

dff2msl - Convert a Denovo flux file into a mesh source lite.

Intended use: Take Denovo fission source information stored in a *.dff file and convert it to a mesh source lite file (*.msl) to be used as a KENO starting source, nst=9.

Input: A Denovo flux (*.dff) file

Output: A mesh source lite (*.msl) file

Example:

```
=dff2msl
"wishfulThinking.dff"
!
e
x
i
s
t
i
n
g
D
e
n
o
v
o
f
l
u
x
f
i
l
e
```

(continues on next page)

(continued from previous page)

```
"startingSource.msl"
!
m
e
s
h
s
o
u
r
c
e
l
i
t
e
f
i
l
e
end
```

dffBinOp - Binary operation of Denovo flux files: sum, difference, product and ratio.

Intended use: Apply simple math to the results stored in Denovo flux files.

Input: The first flux file, the operator: add (or sum, +), subtract (or difference, -), multiply (or product, x, *), or divide (or ratio, ÷, "/"), the second flux file name, and the name of the resulting flux file

Output: A Denovo flux file

Notes: Flux files need to have the same grid structure and number of groups. When using the / (slash) for division, enclose it in quotes ("/").

Example:

```
=dffBinOp
"neutron.dff"
!
f
i
r
s
t
o
p
e
r
a
n
d

d
i
v
i
d
e
!
```

(continues on next page)

```
o
p
e
r
a
t
i
```

(continued from previous page)

```
"total.dff"
!
s
e
c
o
n
d
o
p
e
r
a
n
d
"ratio.dff"
!
o
u
t
p
u
t
f
i
l
e
n
a
m
e
end
```

dffDisp - Display the basics of a Denovo flux file.

Input: A Denovo flux (*.dff) file

Output: Some of the basic details of the Denovo flux file

Example:

```
=dffDisp
"fluxes.dff"
!
e
x
i
s
t
i
n
g
D
e
n
o
v
o
```

(continues on next page)

```
f
l
u
x
f
i
l
```

(continued from previous page)

```
end
```

dffExpand - Expand a space-only Denovo flux file by an energy function.

Input: A Denovo flux (*.dff) file (with a single group - a space-only function), one or more particle types, and an energy function for each

Output: A full space/energy Denovo flux file

Example:

```
=dffExpand
"spatialFluxes.dff"
!
e
x
i
s
t
i
n
g
D
e
n
o
v
o
f
l
u
x
f
i
l
e
(
s
i
n
g
l
e
g
r
o
u
p
)
2
!
n
u
m
b
e
r
o
f
p
a
r
t
i
c
l
```

(continues on next page)

(continued from previous page)

```
1
!
p
a
r
t
i
c
l
e
t
y
p
e
(1
-
n
e
u
t
r
o
n
, 2
-
p
h
o
t
o
n
)
27
!
n
u
m
b
e
r
o
f
b
i
n
s
i
n
b
i
n
n
e
d
h
i
s
t
o
g
r
a
m
d
```

(continues on next page)

(continued from previous page)

```
2
.00000
E
+07 3
.0658021
E
-09
!
E
_1
a
m
o
u
n
t
_1
6
.37630
E
+06 6
.9767163
E
-09
!
E
_2
a
m
o
u
n
t
_2
3
.01190
E
+06 1
.1495182
E
-08
!
E
_3
a
m
o
u
n
t
_3

.
.
.
.
.
.
```

(continues on next page)

(continued from previous page)

```
3
.00000
E
-02 1
.7127996
E
-04
!
E
_26
a
m
o
u
n
t
_26
1
.00000
E
-02 3
.0910611
E
-04
!
E
_27
a
m
o
u
n
t
_27
1
.00000
E
-05
!
E
_28
2
!
p
a
r
t
i
c
l
e
t
y
p
e
(1
-
n
e
u
t
r
o
n
```

(continues on next page)

(continued from previous page)

```
19
!
n
u
m
b
e
r
o
f
b
i
n
s
i
n
b
i
n
n
e
d
h
i
s
t
o
g
r
a
m
d
i
s
t
r
i
b
u
t
i
o
n
2
.00
E
+07 0
.0
!
E
_1
a
m
o
u
n
t
```

_1

(continues on next page)

(continued from previous page)

```
1
.00
E
+07 0
.0
!
E
_2
a
m
o
u
n
t
_2
8
.00
E
+06 0
.0
!
E
_3
a
m
o
u
n
t
_3

.
.
.
.
.
.
1
.00
E
+05 0
.0
!
E
_17
a
m
o
u
n
t
_17
4
.50
E
+04 0
.0
```

(continues on next page)

```
!
E
_18
a
m
o
u
```

(continued from previous page)

```
1
.00
E
+04
!
E
_19
"expanded.dff"
!
n
e
w
D
e
n
o
v
o
f
l
u
x
f
i
l
e
end
```

dffFilter - Perform various filters on a Denovo flux file.

Intended use: Keep fluxes in a *.dff file where the flux or response meets a specified criterion.

Input: A Denovo flux file name, filter type, filter options, the output file name

Output: A Denovo flux file

Notes: There are three basics types of filters: 0) flattening filter, 1) high-pass filter, 2) low-pass filter. For types 1 and 2, the criteria could be a computed response. The input list changes depending on the filter type and whether a response function is included. For no response function, use 0 for the number of groups. A flattening filter turns any positive value into a value of "1.0".

Examples:

```
=dffFilter
"some.dff"
!
i
n
p
u
t
D
e
n
o
v
o
f
l
u
x
f
i
l
e
n
```

(continues on next page)

(continued from previous page)

```
0
!
f
i
l
t
e
r
t
y
p
e
"flattened.dff"
!
o
u
t
p
u
t
D
e
n
o
v
o
f
l
u
x
f
i
l
e
n
a
m
e
end

=dffFilter
"some.dff"
!
i
n
p
u
t
D
e
n
o
v
o
f
l
u
x
f
i
l
e
n
a
```

(continues on next page)

(continued from previous page)

```
2
!
f
i
l
t
e
r
t
y
p
e
10
.0
!
m
a
x
i
m
u
m
v
a
l
u
e
0
!
n
u
m
b
e
r
o
f
g
r
o
u
p
s
f
o
r
r
e
s
p
o
n
s
e
f
u
n
c
t
i
o
n
```

(continues on next page)

(continued from previous page)

```
"simpleFiltered.dff"
!
o
u
t
p
u
t
D
e
n
o
v
o
f
l
u
x
f
i
l
e
n
a
m
e
end

=dffFilter
"some.dff"
!
i
n
p
u
t
D
e
n
o
v
o
f
l
u
x
f
i
l
e
n
a
m
e
1
!
f
i
l
t
e
r
t
y
```

(continues on next page)

(continued from previous page)

```
10
.0
!
m
i
n
i
m
u
m
v
a
l
u
e
19
!
n
u
m
b
e
r
o
f
g
r
o
u
p
s
f
o
r
r
e
s
p
o
n
s
e
f
u
n
c
t
i
o
n
1
.1620022
E
-05
!
s
h
```

(continues on next page)

```
o
u
l
d
m
a
t
```

(continued from previous page)

```
8.7445696E-06
7.4596655E-06
6.3505804E-06
5.3994922E-06
4.6016462E-06
3.9522688E-06
3.4588520E-06
3.0130868E-06
2.6200121E-06
2.1944491E-06
1.8269592E-06
1.5149031E-06
1.1595382E-06
8.7044964E-07
6.2187445E-07
3.7080767E-07
2.6877788E-07
5.9327226E-07
"respFiltered.dff"
!
o
u
t
p
u
t
D
e
n
o
v
o
f
l
u
x
f
i
l
e
n
a
m
e
end
```

dffFix - Fix the zero and negative values in a Denovo flux file.

Intended use: Replace zero or negative values with nearest good neighboring value. Checks previous group, previous x voxel, previous y voxel, then previous z voxel.

Input: A Denovo flux file

Output: A new Denovo flux file

Example:

```
=dffFix
"original.dff"
!
e
x
i
s
t
i
n
g
D
e
n
o
v
o
f
l
u
x
f
i
l
e
"repaired.dff"
!
n
e
w
D
e
n
o
v
o
f
l
u
x
f
i
l
e
end
```

dffInt - Integrate a single particle type from a Denovo flux file.

Input: A Denovo flux file, which particle type to integrate (1-neutron, 2-photon), and the filename of the resulting integrated file

Output: A single-group Denovo flux file

Example:

```
=dffInt
"coupled.dff"
!
e
```

(continues on next page)

```
x
i
s
t
i
n
g
```

(continued from previous page)

```
2
!
p
a
r
t
i
c
l
e
t
y
p
e
"photonTotal.dff"
!
n
e
w
D
e
n
o
v
o
f
l
u
x
f
i
l
e
(
s
i
n
g
l
e
g
r
o
u
p
)
end
```

dffInv - Invert the values in a Denovo flux file.

Input: A Denovo flux file

Output: A Denovo flux file

Notes: Only non-zero values are inverted

Example:

```
=dffInv
"fluxes.dff"
!
e
x
i
s
t
i
n
g
D
e
n
o
v
o
f
l
u
x
f
i
l
e
"inverted.dff"
!
n
e
w
D
e
n
o
v
o
f
l
u
x
f
i
l
e
end
```

dffMult - Multiply a Denovo flux file by a constant factor.

Intended use: source strength change, change in units, etc.

Input: A Denovo flux file and a constant factor

Output: A Denovo flux file

Example:

```
=dffMult
"fluxes.dff"
!
e
x
i
s
t
i
n
g
```

(continues on next page)

(continued from previous page)

```
10000
.0
!
c
h
a
n
g
e
u
n
i
t
s
f
r
o
m
(
/
c
m
^2
/
s
)
t
o
(
/
m
^2
/
s
)
"multiplied.dff"
!
n
e
w
D
e
n
o
v
o
f
l
u
x
f
i
l
e
end
```

dffPull - Pull fluxes from certain voxels out of a Denovo flux file.

Intended use: Get energy-dependent fluxes for certain locations from a flux file.

Input: A Denovo flux file and a list of positions and/or voxels

Output: Listing of energy-dependent fluxes from each desired location to an ASCII text file

Notes: Can pull fluxes either by a physical coordinate position or by voxel indices.

Example:

```
=dffPull
"fluxes.dff"
!
f
i
l
e
w
i
t
h
t
h
e
s
c
a
l
a
r
f
l
u
x
e
s
y
o
u
w
a
n
t

n
!
n
u
m
b
e
r
o
f
x
,
y
,
z
p
o
i
n
t
s
t
o
```

(continues on next page)

(continued from previous page)

```
x
_1
y
_1
z
_1
!
c
o
o
r
d
i
n
a
t
e
s
o
f
p
o
i
n
t 1

x
_1
y
_2
z
_2
!
c
o
o
r
d
i
n
a
t
e
s
o
f
p
o
i
n
t 2

.
.
.
```

(continues on next page)

```
x
_
n
y
_
n
z
```

(continued from previous page)

```
m
!
n
u
m
b
e
r
o
f
i
,
j
,
k
v
o
x
e
l
s
t
o
p
u
l
l

i
_1
j
_1
k
_1
!
i
n
d
i
c
e
s
o
f
v
o
x
e
l 1

i
_2
j
_2
k
_2
!
i
n
d
i
c
e
```

(continues on next page)

(continued from previous page)

```
.
.
.

i
_
m
j
_
m
k
_
m
!
i
n
d
i
c
e
s
o
f
v
o
x
e
l
m
"outputName.txt"
!
n
a
m
e
o
f
o
u
t
p
u
t
t
e
x
t
f
i
l
e
=end
```

dffResp - Apply a response function to scalar fluxes in a Denovo flux file.

Intended use: Compute group-wise dose or reaction rates by combining a response function with the scalar fluxes. This can be done for every particle type in the flux file or a single specific particle type.

Input: A Denovo flux file, particle indicator and a group-wise response function

Output: A Denovo flux file

Notes: 0-all particles, 1-neutron, 2-photon

Example:

```
=dffResp
"fluxes.dff"
!
e
x
i
s
t
i
n
g
c
o
u
p
l
e
d
D
e
n
o
v
o
f
l
u
x
f
i
l
e
1
!
k
e
e
p
o
n
l
y
n
e
u
t
r
o
n
i
n
f
o
r
m
a
t
i
o
```

(continues on next page)

(continued from previous page)

```
200
!
n
u
m
b
e
r
o
f
b
i
n
s
i
n
r
e
s
p
o
n
s
e
2
.2675480
E
-04
!
r
e
s
p
o
n
s
e
g
r
o
u
p 1
2
.2283355
E
-04
!
r
e
s
p
o
n
s
e
g
r
```

(continues on next page)

```
o
u
p 2
```

(continued from previous page)

```
2
.1878259
E
-04
!
r
e
s
p
o
n
s
e
g
r
o
u
p 3

.
.
.
3
.6748440
E
-06
!
r
e
s
p
o
n
s
e
g
r
o
u
p
n
b
i
n
s
-2
3
.6748443
E
-06
!
r
e
s
p
o
n
```

(continues on next page)

```
s
e
g
r
o
u
p
```

(continued from previous page)

```
3
.6748436
E
-06
!
r
e
s
p
o
n
s
e
g
r
o
u
p
n
b
i
n
s
"doses.dff"
!
n
e
w
(
s
m
a
l
l
e
r
)
D
e
n
o
v
o
f
l
u
x
f
l
e
end
```

or

```
=dffResp
"fluxes.dff"
!
e
x
i
s
t
i
n
```

(continues on next page)

(continued from previous page)

```
0
!
k
e
e
p
a
l
l
p
a
r
t
i
c
l
e
s
i
n
f
o
r
m
a
t
i
o
n
46
!
n
u
m
b
e
r
o
f
b
i
n
s
i
n
r
e
s
p
o
n
s
e
1
.6151395
E
-04
```

(continues on next page)

```
!
r
e
s
p
o
n
```

(continued from previous page)

```
1
.4451494
E
-04
!
r
e
s
p
o
n
s
e
g
r
o
u
p 2
1
.2703618
E
-04
!
r
e
s
p
o
n
s
e
g
r
o
u
p 3

.
.
.
3
.6748447
E
-06
!
r
e
s
p
o
n
s
e
g
r
o
u
```

(continues on next page)

```
p 27
,
1
a
s
t
n
```

(continued from previous page)

```
1
.1620022
E
-05
!
r
e
s
p
o
n
s
e
g
r
o
u
p 28
,
f
i
r
s
t
p
h
o
t
o
n
8
.7445696
E
-06
!
r
e
s
p
o
n
s
e
g
r
o
u
p 29
7
.4596655
E
-06
!
r
e
s
p
```

(continues on next page)

```
o
n
s
e
g
r
o
```

(continued from previous page)

```
.
.
.
5
.9327226
E
-07
!
r
e
s
p
o
n
s
e
g
r
o
u
p 46
,
l
a
s
t
p
h
o
t
o
n
"doses.dff"
!
n
e
w
D
e
n
o
v
o
f
l
u
x
f
i
l
e
end
```

dffSplit - Split off a single particle type from a Denovo flux file.

Intended use: Make a flux file containing a single particle type from another Denovo flux file.

Input: A Denovo flux file and a particle type

Output: A (smaller) Denovo flux file

Notes: 1-neutron, 2-photon

Example:

```
=dffSplit
"coupled.dff"
!
e
x
i
s
t
i
n
g
D
e
n
o
v
o
f
l
u
x
f
i
l
e
2
!
p
a
r
t
i
c
l
e
t
y
p
e
"photons.dff"
!
n
e
w
(
s
m
a
l
l
e
r
)
D
e
n
o
v
o
```

(continues on next page)

(continued from previous page)

```
end
```

3.4 Utilities for working with DENOVO *.varscl (a TORT format) files

These utilities include the following:

vs2dff	Convert a varscl file into a Denovo flux file.
vsAdder	Add two TORT *.varscl files together into one *.varscl file.
vsBinOp	Binary operation of TORT *.varscl files: sum, difference, product and ratio.
vsDisp	Display the basic contents of a TORT *.varscl file.
vsFilter	Perform various filters on a TORT *.varscl file.
vsInt	Integrate a single particle type from a TORT *.varscl file.
vsInv	Invert the values in a TORT *.varscl file.
vsMult	Multiply a TORT *.varscl file by a constant factor.
vsPull	Pull fluxes from certain voxels out of a TORT *.varscl file.
vsReGrp	Regroup a TORT *.varscl file.
vsResp	Apply a response function to scalar fluxes in a TORT *.varscl file.
vsSplit	Split off part of a TORT *.varscl file into a separate *.varscl file.

These utilities work with the *.varscl files produced with SCALE 6 and SCALE 6.1. The *.varscl format (a TORT format) is a single precision, binary format that has been replaced with the double precision, binary *.dff file (Denovo flux file) in SCALE 6.2. SCALE 6 and SCALE 6.1 users can request the executable binaries for these utilities by sending an email to scaleHelp@ornl.gov.

vs2dff - Convert a varscl file into a Denovo flux file.

Intended use: Convert a varscl file (used in previous versions of MAVRIC) into a Denovo flux file (introduced in SCALE 6.2).

Input: The *varscl file name, whether or not it is an adjoint flux, and the filename for the resulting denovoFluxfile

Output: A binary (stream) denovoFluxFile

Example:

```
=vs2dff
"mavricUtilities3.adjoint.varscl"
!
t
h
e
T
O
R
T
v
a
r
s
c
l
f
i
l
```

(continues on next page)

```
e
```

(continued from previous page)

```
t
r
u
e
!
i
t
i
s
a
n
a
d
j
o
i
n
t
f
l
u
x
"mavricUtilities3.adjoint.dff"
!
n
e
w
d
e
n
o
v
o
F
l
u
x
F
i
l
e
end
```

vsAdder - Add two TORT *.varscl files together into one *.varscl file.

Intended use: Beta versions of MAVRIC used TORT and GRTUNC-3D and could add the *.varscl files from each together before using them to create importance maps. MAVRIC now uses Denovo and no longer needs to add separate GRTUNC/TORT files. This utility is designed for people wishing to use the older files with the latest MAVRIC.

Input: Two *.varscl file names, typically one from GRTUNC-3D and the other from TORT, the filename of the added file, whether you want lots of output displayed ("true" or "false") and whether or not there is a minimum value of flux to use. If so, it is then listed.

Output: A single *.varscl with the specified name

Notes: Addition is commutative, but not all varscl files are created equal. Do not mix up the GRTUNCL and the TORT files. GRTUNCL3D does not fill in the header info quite right, so the added varscl file takes header info only from the

TORT varscl file.

Example:

```
=vsAdder

"
/
s
o
m
e
/
p
a
t
h
/
p
r
o
b
l
e
m
.
g
t
u
n
c
.
a
d
j
o
i
n
t
.
v
a
r
s
c
l
"

"
/
s
o
m
e
/
p
a
t
h
```

(continues on next page)

```
/
p
r
o
b
l
e
```

(continued from previous page)

```
"
t
o
t
a
l
.
v
a
r
s
c
l
"

f

t
1.0e-25
end

=shell

c
p
t
o
t
a
l
.
v
a
r
s
c
l
$
{
R
T
N
D
I
R
}
/
t
o
t
a
l
.
v
a
r
s
c
l
```

(continues on next page)

(continued from previous page)

```
end
```

vsBinOp - Binary operation of TORT *.varscl files: sum, difference, product and ratio.

Intended use: Apply simple math to the results stored in TORT *.varscl files.

Input: The first flux file, the operator: add (or sum, +), subtract (or difference, -), multiply (or product, x, *), and divide (or ratio, ÷, "/"), the second flux file name, and the name of the resulting flux file

Output: A TORT *.varscl file

Notes: Flux files need to have the same grid structure and number of groups. When using the / (slash) for division, enclose it in quotes ("/").

Example:

```
=vsBinOp
"neutron.varscl"
!
f
i
r
s
t
o
p
e
r
a
n
d

f
a
l
s
e
!
a
r
e
t
h
e
s
e
a
d
j
o
i
n
t
f
i
l
e
s
?
```

(continues on next page)

(continued from previous page)

```
d
i
v
i
d
e
!
o
p
e
r
a
t
i
o
n
"total.varscl"
!
s
e
c
o
n
d
o
p
e
r
a
n
d
"ratio.varscl"
!
o
u
t
p
u
t
f
i
l
e
n
a
m
e
end
```

vsDisp - Display the basic contents of a TORT *.varscl file.

Input: A TORT *.varscl file name and adjoint flag

Output: Text display

Examples:

```
=vsDisp
"some.varscl"
!
i
n
p
u
t
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
n
a
m
e

f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
v
a
r
s
c
l
?
```

(continues on next page)

(continued from previous page)

```
end

=vsDisp
"some.varscl"
!
i
n
p
u
t
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
n
a
m
e

a
d
j
o
i
n
t
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
v
a
r
s
c
l
```

(continues on next page)

(continued from previous page)

```
end
```

vsFilter - Perform various filters on a TORT *.varscl file.

Intended use: Keep fluxes in a *.varscl file where the flux or response meets a specified criterion.

Input: A TORT *.varscl file name, filter type, filter options, the output file name

Output: A TORT *.varscl file

Notes: There are three basics types of filters: 0) flattening filter, 1) high-pass filter, 2) low-pass filter. For types 1 and 2, the criteria could be a computed response. The input list changes depending on the filter type and whether a response function is included. For no response function, use 0 for the number of groups.

Examples:

```
=vsFilter
"some.varscl"
!
i
n
p
u
t
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
n
a
m
e

f
a
l
s
e
!
i
s
t
h
i
s
a
n
```

(continues on next page)

```
a
d
i
o
i
n
t
```

(continued from previous page)

```
0
!
f
i
l
t
e
r
t
y
p
e
"flattened.varscl"
!
o
u
t
p
u
t
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
n
a
m
e
end

=vsFilter
"some.varscl"
!
i
n
p
u
t
T
O
R
T
*
.
v
a
r
s
c
l
f
i
```

(continues on next page)

(continued from previous page)

```
f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
v
a
r
s
c
l
?
2
!
f
i
l
t
e
r
t
y
p
e
10
.0
!
m
a
x
i
m
u
m
v
a
l
u
e
0
```

(continues on next page)

```
!
n
u
m
b
e
r
```

(continued from previous page)

```
"simpleFiltered.varscl"
!
o
u
t
p
u
t
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
n
a
m
e
end

=vsFilter
"some.varscl"
!
i
n
p
u
t
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
n
a
m
e
```

(continues on next page)

(continued from previous page)

```
f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
v
a
r
s
c
l
?
1
!
f
i
l
t
e
r
t
y
p
e
10
.0
!
m
i
n
i
m
u
m
v
a
l
u
e
19
!
n
u
m
b
e
r
```

(continues on next page)

(continued from previous page)

```
1
.1620022
E
-05
!
s
h
o
u
l
d
m
a
t
c
h
t
o
t
a
l
g
r
o
u
p
s
i
n
f
i
l
e
8.7445696E-06
7.4596655E-06
6.3505804E-06
5.3994922E-06
4.6016462E-06
3.9522688E-06
3.4588520E-06
3.0130868E-06
2.6200121E-06
2.1944491E-06
1.8269592E-06
1.5149031E-06
1.1595382E-06
8.7044964E-07
6.2187445E-07
3.7080767E-07
2.6877788E-07
5.9327226E-07
"respFiltered.varscl"
!
o
u
t
p
u
t
T
O
R
T
*
```

(continues on next page)

(continued from previous page)

vsInt - Integrate a single particle type from a TORT *.varscl file.

Input: A TORT *.varscl file

Output: A single-group TORT *.varscl file

Example:

```
=vsInt
"coupled.varscl"
!
e
x
i
s
t
i
n
g
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e

f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
f
i
l
e
?
```

(continues on next page)

(continued from previous page)

```
2
!
p
a
r
t
i
c
l
e
t
y
p
e
(0
-
a
l
l
, 1
-
n
e
u
t
r
o
n
, 2
-
p
h
o
t
o
n
)
"photonTotal.varscl"
!
n
e
w
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
(
s
t
r
i
n
g
l
```

(continues on next page)

(continued from previous page)

```
end
```

vsInv - Invert the values in a TORT *.varscl file.

Input: A TORT *.varscl file

Output: A TORT *.varscl file

Notes: Only non-zero values are inverted

Example:

```
=vsInv
"fluxes.varscl"
!
e
x
i
s
t
i
n
g
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e

f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
f
i
l
e
?
```

(continues on next page)

(continued from previous page)

```
"inverted.varscl"
!
n
e
w
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
end
```

vsMult - Multiply a TORT *.varscl file by a constant factor.

Intended use: source strength change, change in units, etc.

Input: A TORT *.varscl file and a constant factor

Output: A TORT *.varscl file

Example:

```
=vsMult
"fluxes.varscl"
!
e
x
i
s
t
i
n
g
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
```

(continues on next page)

(continued from previous page)

```
f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
f
i
l
e
?
10000
.0
!
c
h
a
n
g
e
u
n
i
t
s
f
r
o
m
(
/
c
m
^2
/
s
)
t
o
(
/
m
^2
/
s
)
```

(continues on next page)

(continued from previous page)

```
"multiplied.varscl"
!
n
e
w
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
end
```

vsPull - Pull fluxes from certain voxels out of a TORT *.varscl file.

Intended use: Get energy-dependent fluxes for certain locations from a flux file.

Input: A TORT *.varscl file and a list of positions and/or voxels

Output: Listing of energy-dependent fluxes from each desired location to an ASCII text file

Notes: Can pull fluxes either by a physical coordinate position or by voxel indices.

Example:

```
=vsPull
"fluxes.varscl"
!
f
i
l
e
w
i
t
h
t
h
e
s
c
a
l
a
r
f
l
u
x
```

(continues on next page)

```
e
s
y
o
u
w
a
```

(continued from previous page)

```
f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
f
i
l
e
?

n
!
n
u
m
b
e
r
o
f
x
,
y
,
z
p
o
i
n
t
s
t
o
p
u
l
l

x
_1
y
_1
z
_1
!
c
```

(continues on next page)

(continued from previous page)

```
x
_1
y
_2
z
_2
!
c
o
o
r
d
i
n
a
t
e
s
o
f
p
o
i
n
t 2

.
.
.

x
_
n
y
_
n
z
_
n
!
c
o
o
r
d
i
n
a
t
e
s
o
f
p
o
i
n
t
n
```

(continues on next page)

(continued from previous page)

```
m
!
n
u
m
b
e
r
o
f
i
,
j
,
k
v
o
x
e
l
s
t
o
p
u
l
l

i
_1
j
_1
k
_1
!
i
n
d
i
c
e
s
o
f
v
o
x
e
l 1

i
_2
j
_2
k
_2
!
i
n
d
i
c
e
```

(continues on next page)

(continued from previous page)

```
.
.
.

i
_
m
j
_
m
k
_
m
!
i
n
d
i
c
e
s
o
f
v
o
x
e
l
m
"outputName.txt"
!
n
a
m
e
o
f
o
u
t
p
u
t
t
e
x
t
f
i
l
e
end
```

vsReGrp - Regroup a TORT *.varscl file.

Input: A TORT *.varscl file and adjoint flag, then a list of how the new groups should be formed from the old groups

Output: A smaller TORT *.varscl file

Example:

```
=vsReGrp
"coupled.varscl"
!
e
x
i
s
t
i
n
g
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e

f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
f
i
l
e
?
```

(continues on next page)

(continued from previous page)

```
27
!
n
u
m
b
e
r
o
f
n
e
u
t
r
o
n
g
r
o
u
p
s
i
n
f
i
l
e
1
!
n
e
w
g
r
o
u
p
a
s
s
i
g
n
m
e
n
t
f
o
r
e
a
c
h
1
```

(continues on next page)

```
!
e
x
i
s
t
i
```

(continued from previous page)

```
1
!
m
u
s
t
s
t
a
r
t
w
i
t
h
o
n
e
2
!
e
a
c
h
e
n
t
r
y
i
s
s
a
m
e
a
s
l
a
s
t
o
r

.
.
.
!
i
n
c
r
e
a
s
e
s
b
y 1
```

(continues on next page)

(continued from previous page)

```
8
!
n
e
w
g
r
o
u
p
a
s
s
i
g
n
m
e
n
t
f
o
r
n
e
u
t
r
o
n
g
r
o
u
p 27
19
!
n
u
m
b
e
r
o
f
p
h
o
t
o
n
g
r
o
u
p
s
i
n
f
i
l
e
```

(continues on next page)

(continued from previous page)

```
1
!
n
e
w
g
r
o
u
p
a
s
s
i
g
n
m
e
n
t
f
o
r
e
a
c
h
1
!
e
x
i
s
t
i
n
g
p
h
o
t
o
n
g
r
o
u
p
1
!
m
u
s
t
s
t
a
r
t
w
i
t
h
o
```

(continues on next page)

(continued from previous page)

```
2
!
e
a
c
h
e
n
t
r
y
i
s
s
a
m
e
a
s
l
a
s
t
o
r

.
.
.
!
i
n
c
r
e
a
s
e
s
b
y 1
4
!
n
e
w
g
r
o
u
p
a
s
s
i
g
n
m
e
n
t
f
o
r
```

(continues on next page)

(continued from previous page)

```
"smaller.varscl"
!
n
e
w
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
n
a
m
e
end
```

vsResp - Apply a response function to scalar fluxes in a TORT *.varscl file.

Intended use: Compute group-wise dose or reaction rates by combining a response function with the scalar fluxes.

Input: A TORT *.varscl file and a group-wise response function

Output: A TORT *.varscl file

Example:

```
=vsResp
"fluxes.varscl"
!
e
x
i
s
t
i
n
g
c
o
u
p
l
e
d
T
O
R
T
*
.
v
a
r
s
c
```

(continues on next page)

(continued from previous page)

```
f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
f
i
l
e
?
200
!
n
u
m
b
e
r
o
f
b
i
n
s
i
n
r
e
s
p
o
n
s
e
2
.2675480
E
-04
!
r
e
s
p
o
n
s
e
```

(continues on next page)

(continued from previous page)

```
2
.2283355
E
-04
!
r
e
s
p
o
n
s
e
g
r
o
u
p 2
2
.1878259
E
-04
!
r
e
s
p
o
n
s
e
g
r
o
u
p 3

.
.
.
3
.6748440
E
-06
!
r
e
s
p
o
n
s
e
g
r
o
u
p 198
```

(continues on next page)

(continued from previous page)

```
3
.6748443
E
-06
!
r
e
s
p
o
n
s
e
g
r
o
u
p 199
3
.6748436
E
-06
!
r
e
s
p
o
n
s
e
g
r
o
u
p 200
"doses.varscl"
!
n
e
w
(
s
m
a
l
l
e
r
)
D
e
n
o
v
o
f
l
u
x
r
l
e
```

(continues on next page)

(continued from previous page)

```
end
```

vsSplit - Split off part of a TORT *.varscl file into a separate *.varscl file.

Intended use: Make a flux file containing a single particle type from another TORT *.varscl file.

Input: A TORT *.varscl file and a particle type

Output: A (smaller) TORT *.varscl file

Example:

```
=vsSplit
"coupled.varscl"
!
e
x
i
s
t
i
n
g
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e

f
a
l
s
e
!
i
s
t
h
i
s
a
n
a
d
j
o
i
n
t
f
i
l
e
?
```

(continues on next page)

(continued from previous page)

```
2
!
p
a
r
t
i
c
l
e
t
y
p
e
(1
-
n
e
u
t
r
o
n
, 2
-
p
h
o
t
o
n
)
"photons.varscl"
!
n
e
w
(
s
m
a
l
l
e
r
)
T
O
R
T
*
.
v
a
r
s
c
l
f
i
l
e
```

(continues on next page)

(continued from previous page)

```
end
```

3.5 Miscellaneous utilities

These utilities include the following:

dsi2asc	Convert a Denovo simple input (*.dsi) from binary to ASCII.
dsiDisp	Display the basics of a Denovo simple input file.
dso2msl	Use a Denovo spatial output to create a mesh source lite.
dsoDisp	Display the basics of a Denovo spatial output file.
mim2wwinp	Convert a mesh importance map into an MCNP weight window file.
mimDisp	Display the basics of a mesh importance map (*.mim) file.
mimNorm	Normalize a mesh importance map to a given location/energy.
msmDisp	Display the basics of a mesh source map (*.msm) file.

dsi2asc - Convert a Denovo simple input (*.dsi) from binary to ASCII.

Intended use: Check a Denovo input file for correctness.

Input: Names of original binary Denovo simple input (*.dsi) file and the desired ASCII text file

Output: Human-readable form of the Denovo input file

Example:

```
=dsi2asc
"input.dsi"
!
D
e
n
o
v
o
s
i
m
p
l
e
i
n
p
u
t
f
i
l
e
(
b
i
n
a
r
y
)
```

(continues on next page)

(continued from previous page)

```
"ascii.txt"
!
n
e
w
a
s
c
i
i
t
e
x
t
f
i
l
e
end
```

dsiDisp - Display the basics of a Denovo simple input file.

Input: A Denovo simple input (*.dsi) file

Output: Some of the basic details of the Denovo simple input file

Example:

```
=dsiDisp
"godiva.dsi"
!
e
x
i
s
t
i
n
g
D
e
n
o
v
o
s
i
m
p
l
e
i
n
p
u
t
f
i
l
e
```

(continues on next page)

(continued from previous page)

```
end
```

dso2msl - Use a Denovo spatial output to create a mesh source lite.

Input: A *.dso file is made of three-dimensional data sets called fields. Which field to convert? 1-n: convert that field 0: convert sum of all fields

Output: A mesh source lite (*.msl) file for KENO-VI.

Example:

```
=dso2msl
"fisSource.dso"
!
D
e
n
o
v
o
s
p
a
t
i
a
l
o
u
t
p
u
t
f
i
l
e
w
i
t
h
m
a
n
y
f
i
e
l
d
s
1
!
w
h
i
c
h
f
i
e
l
d
t
o
```

(continues on next page)

(continued from previous page)

```
"test.msl"
!
n
e
w
M
o
n
a
c
o
m
e
s
h
s
o
u
r
c
e
l
i
t
e
end
```

dsoDisp - Display the basics of a Denovo spatial output file.

Input: A Denovo spatial output (*.dsi) file

Output: Some of the basic details of the Denovo spatial output file

Example:

```
=dsoDisp
"godiva.dso"
!
e
x
i
s
t
i
n
g
D
e
n
o
v
o
s
p
a
t
i
a
l
o
u
t
p
u
t
```

(continues on next page)

(continued from previous page)

```
end
```

mim2wwinp - Convert a mesh importance map into an MCNP weight window file.

Intended Use: To create an MCNP weight window file from a Monaco mesh importance map file outside of a MAVRIC calculation. Monaco mesh importance map files store target weights, but MCNP wwinp files store lower weight bounds. To convert, the user needs to supply the windowRatio, r (the ratio of the upper weight bound for splitting to the lower weight bound for roulette). Target weights, t, are the average of the upper, u, and lower, l, weight window bounds, so l=2t/(r+1). For example, for a Monaco target weight of 1.0 and a windowRatio of 10.0, the MCNP lower weight bound will be l=2(1.0)/(10.0+1)=0.1818. To reduce the size of the map, the user can specify which neutron and photon groups to store in the new file. If the last group is less than the first group, no groups of that particle will be stored.

Input:

Line 1: filename of the Monaco mesh importance map file

Line 2: windowRatio (>1.0)

Line 3: first_neutron_group last_neutron_group

Line 4: first_photon_group last_photon_group

Line 5: filename of the MCNP weight window input file

Output: The resulting weight window input file stored with the desired filename

Notes: Geometry information in the Monaco mesh importance map file is lost since the MCNP wwinp format does not support it.

Example:

```
=
m
i
m2
w
w
i
n
p
"/scale/smplprbs/mavric.graphiteCADIS.mim"
!
i
m
p
o
r
t
a
n
c
e
m
a
p
19
.0
!
w
i
n
d
o
w
r
```

(continues on next page)

(continued from previous page)

```
5 22
!
s
a
v
e
n
g
r
o
u
p
s 5
-22
19 1
!
s
a
v
e
n
o
p
g
r
o
u
p
s
"/scale/test9/testmimww.wwinp"
!
n
e
w
f
i
l
e
end
```

mimDisp - Display the basics of a mesh importance map file.

Input: A mesh importance map (*.mim) file

Output: Some of the basic details of mesh importance map file

Example:

```
=mimDisp
"the.mim"
!
e
x
i
s
t
i
n
g
m
e
s
h
i
m
```

(continues on next page)

(continued from previous page)

```
end
```

mimNorm - Normalize a mesh importance map to a given location/energy.

Input: A mesh importance map (*.mim) file, a location (x, y, z), a particle type and energy, and a filename for the normalized map file. Use 1 for neutron and 2 for photon. Energy should be in eV. The new importance map file will be normalized such that the given location/energy has a target weight of 1. If a particle type or energy is 0, then the energy group with the minimum non-zero target value at the given location will be the group that is set to 1.0 in the new file. (This option is similar to the MCNP weight window generator.)

Output: A mesh importance map file

Example:

```
=mimNorm
"the.mim"
!
e
x
i
s
t
i
n
g
m
e
s
h
i
m
p
o
r
t
a
n
c
e
m
a
p
f
i
l
e
27
.5
-16
.5 32
.0
!
l
o
c
a
t
i
```

(continues on next page)

```
o
n
```

(continued from previous page)

```
1 1
.0
e6
!
n
e
u
t
r
o
n
, 1
M
e
V
"normed.mim"
!
n
e
w
f
i
l
e
t
h
a
t
i
s
n
o
r
m
a
l
i
z
e
d
end
```

msmDisp - Display the basics of a mesh source map file.

Input: A mesh source map (*.msm) file

Output: Some of the basic details of mesh source map file

Example:

```
=msmDisp
"the.msm"
!
e
x
i
s
t
```

(continues on next page)

```
i
n
g
m
e
s
h
```

(continued from previous page)

CHAPTER

FOUR

MAVRIC APPENDIX C: ADVANCED FEATURES

This appendix contains information on several advanced features that are still under development or are non-standard use of the MAVRIC sequence.

4.1 Alternate normalization of the importance map and biased source

The importance map and biased source implemented in MAVRIC are only functions of space and energy. The importance for a specific location and energy represents the average over all directions. For applications involving a collimated beam source, a space/energy importance map may not be representative of the true importance of the particles as they stream away from the source.

As an example, consider a 14.1 MeV active interrogation beam source 1 meter from a small spherical boat containing illicit nuclear material. The objective is to compute the fission rate in the nuclear material. To create the biasing parameters, an adjoint source is located within the nuclear material and the resulting importance map is shown in Fig. 4.1. Note that in both the air and water, the importances change with distance from the ship, but for the beam source, the importance (to causing a fission in the nuclear material) anywhere along the beam should be the same, since there is little chance a 14.1 MeV neutron will interact with the air before striking the ship.

Fig. 4.1: Importance map computed using standard CADIS.

The CADIS algorithm has done exactly what it was supposed to: it made a space/energy importance map and normalized it such that the target weight where the 14.1 MeV source particles are born is 1. The problem with this is that the source particles will stream towards the ship and strike the hull where the target weight is 0.092. Since source particles have little chance of interacting in the air, the weight windows are not used to split the particle as they travel towards the ship. When source particles cross into the ship, they are split by a factor of 11 to match the target weight. For this

example, splitting each particle by a factor of 11 once they strike the ship is not so bad, but for longer distances, this will result in much larger splits. For a polyenergetic source, this could lead to undersampling of the source and could result in higher variances.

To remedy this problem when using beam sources, the normalization of the importance map and biased source should not be done at the source location but instead at the point where the source particles first interact with the ship. The keyword "shiftNormPos x y z" will shift the source normalization position by the amounts x, y, and z when the biased source and importance map are developed. For the Monaco Monte Carlo calculation, the source is returned to its normal position. The source input for the above problem would then be

```
read
 sources

s
r
c 1

t
i
t
l
e
="14.1 DT neutrons - collimated"

s
t
r
e
n
g
t
h=1e30

s
p
h
e
r
e 0
o
r
i
g
i
n
x
=
-195
y
=0
z
=0
(
t
r
u
e
s
o
u
r
```

(continues on next page)


```
e
p
o
s
```

(continued from previous page)

```
e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
(
a
m
o
n
o
-
e
n
e
r
g
e
t
i
c 14
.1
M
e
V
d
i
s
t
r
i
b
u
t
i
o
n
)

d
i
r
e
c
t
i
o
n 1
.0 0
.0 0
.0
```

(continues on next page)

(continued from previous page)

```
d
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=2
(
a 2
°
b
e
a
m
)

s
h
i
f
t
N
o
r
m
P
o
s 107
.7 0
.0 0
.0
(
j
u
s
t
i
n
s
i
d
e
t
h
e
h
u
l
l
)
```

(continues on next page)

(continued from previous page)

```
    end
 src
end
 sources
```

where the shift moves the source position from x = -195 to x = -87.3, just inside the hull. The resulting target weights are shown in Fig. 4.2 The source particles are born with weight 1 in a location with a target weight 10.9. The particle weight is not checked until the particle crosses into the hull, where the target weight is 1.0.

Fig. 4.2: Targets weights using the "shiftNormPos" keyword.

Other options to manipulate the importance map for special situations include the "mapMultiplier=*f*" keyword (in the importanceMap block or the biasing block), which will multiply every target weight by the factor *f*, and the keyword "noCheckAtBirth" in the parameters block will prevent the weight windows from being applied to source particles when they are started. When used in the MAVRIC sequence, the "shiftNormPos" capability automatically adds "noCheckAtBirth" to the Monaco input that is created.

4.2 Importance maps with directional information

In MAVRIC, the CADIS method is implemented in space and energy, but in general, it could also include particle direction as well. This formulation would be the following:

True source:

$$q\left(\overrightarrow{r}, E, \widehat{\Omega}\right)$$

Desired response:

$$\sigma\left(\overrightarrow{r}, E, \widehat{\Omega}\right)$$

Adjoint flux using $q^{+}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) = \sigma\left(\overrightarrow{r}, E, \widehat{\Omega}\right)$**:**

$$\psi^{+}\left(\overrightarrow{r}, E, \widehat{\Omega}\right)$$

Estimate of detector response

$$R = \iiint q\left(\overrightarrow{r}, E, \widehat{\Omega}\right)\ \psi^{+}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) d\,dE\,dV \tag{4.1}$$

Biased source:

$$\widehat{q}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) = \frac{1}{R} q\left(\overrightarrow{r}, E, \widehat{\Omega}\right)\ \psi^{+}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) \tag{4.2}$$

Target weight windows:

$$\overline{w}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) = \frac{R}{\psi^{+}\left(\overrightarrow{r}, E, \widehat{\Omega}\right)} \tag{4.3}$$

For a system using a deterministic method to compute the adjoint fluxes, this completely general, space/energy/angle, approach presents many difficulties in implementation, namely,

a. dealing with the amount of memory required for a $\left(\overrightarrow{r}, E, \widehat{\Omega}\right)$ importance map in memory,

b. interpolating the importance for particle directions in between quadrature angles, and

c. expressing the biased source in a form suitable for a general MC code since the above biased source is, in general, not separable.

4.2.1 Approaches incorporating directional information

Completely general space/energy/angle CADIS is most likely too difficult to implement and may not be necessary for most applications. In most real problems that involve directionally dependent source distributions, the directional dependence is azimuthally symmetric about some reference direction, $\widehat{d}$. The angular distribution, $q_i\left(\widehat{\Omega}\right)$, can be expressed as the product of the uniform azimuthal distribution and a polar distribution about reference direction $\widehat{d_i}$ giving $\frac{1}{2\pi} q_i\left(\widehat{\Omega} \bullet \widehat{d_i}\right)$. The geometric size of these sources tends to be small, allowing each source distribution to be expressed as the product of two separable distributions: $q_i\left(\overrightarrow{r}, E, \widehat{\Omega}\right) \cong q_i\left(\overrightarrow{r}, E\right)\ q_i\left(\widehat{\Omega}\right)$.

What is needed is a CADIS method that (1) can account for the importance of a particle traveling in a certain direction; (2) can be cast as a simple modification of the space/energy CADIS method using $\overline{w}\left(\overrightarrow{r}, E\right)$ and $\widehat{q}\left(\overrightarrow{r}, E\right)$; and (3) is simpler than the full space/angle/energy approach. This can be done starting with the approximation that the angular component of the adjoint flux $\psi^{+}\left(\overrightarrow{r}, E, \widehat{\Omega}\right)$ is separable and symmetric about the average adjoint current direction $\widehat{n}\left(\overrightarrow{r}, E\right)$, such that

$$\psi^{+}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) \cong \phi^{+}\left(\overrightarrow{r}, E\right)\ \frac{1}{2\pi} f\left(\widehat{\Omega} \bullet \widehat{n}\right)\ .$$

This is similar to the AVATAR approach [VRUS97] but with explicitly including the azimuthal distribution so that the standard definition $\int \phi^{+}\left(\overrightarrow{r}, E\right)\ \frac{1}{2\pi} f\left(\widehat{\Omega} \bullet \widehat{n}\right)\ d\widehat{\Omega} = \phi^{+}\left(\overrightarrow{r}, E\right)$ applies. The probability distribution function $f\left(\mu\right)$ describing the shape of the azimuthally symmetric current at $\left(\overrightarrow{r}, E\right)$ has the form of

$$f\left(\mu\right) = \frac{\lambda e}{2\sinh\left(\lambda\right)}\ ,$$

with the single parameter $\lambda\left(\overrightarrow{r}, E\right)$ determined from $\overline{\mu}\left(\overrightarrow{r}, E\right)$, the average cosine of scatter.

From this, we can propose that weight window targets be developed that are inversely proportional to the approximation of the adjoint angular flux:

$$\overline{w}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) = \frac{2\pi\ k}{\phi^{+}\left(\overrightarrow{r}, E\right)\ \ f\left(\widehat{\Omega} \bullet \widehat{n}\right)}\ , \tag{4.4}$$

where k is the constant of proportionality that will be adjusted to make the importance map consistent with the biased source(s). Two methods will be examined here, one without and one with biasing of the source directional dependence.

For both of the methods, the S_N code Denovo was modified to report not only the adjoint scalar fluxes, $\phi^{+}\left(\overrightarrow{r}, E\right)$, but also the adjoint net currents in x, y, and z directions: $J_x\left(\overrightarrow{r}, E\right)$, $J_y\left(\overrightarrow{r}, E\right)$, and $J_z\left(\overrightarrow{r}, E\right)$. These currents are used to find $\widehat{n}\left(\overrightarrow{r}, E\right)$ and $\lambda\left(\overrightarrow{r}, E\right)$. The following methods have been developed so that the standard CADIS routines can be used to compute space/energy quantities of the response per unit source R, the weight window target values $\overline{w}\left(\overrightarrow{r}, E\right)$, and biased source $\widehat{q}\left(\overrightarrow{r}, E\right)$ with just the adjoint scalar fluxes. These quantities are then modified by the directional information.

4.2.2 Directionally dependent weight windows without directional source biasing

It is proposed that the biased source $\widehat{q}\left(\overrightarrow{r}, E, \widehat{\Omega}\right)$ should be proportional to both the true source distribution and the space/energy component of the adjoint flux:

$$\widehat{q}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) = \frac{1}{R}\left[q\left(\overrightarrow{r}, E\right)\ \frac{1}{2\pi} q\left(\widehat{\Omega} \bullet \widehat{d}\right)\right]\ \phi^{+}\left(\overrightarrow{r}, E\right)\ ,$$

where the constant of proportionality, R, is determined by forcing $\widehat{q}\left(\overrightarrow{r}, E, \widehat{\Omega}\right)$ to be a pdf. Since the angular component of the adjoint flux is not included, the directional distribution of the biased source will be exactly the same as the true source. Note that this approach would be exact for cases where no directional biasing could be applied – beam sources.

For multiple sources (each with a probability distribution function $q_i\left(\overrightarrow{r}, E\right)$ and a strength S_i, giving a total source strength of $S = \sum S_i$), the user is required to provide one point in phase space $\left(\overrightarrow{r}_i, E_i, \widehat{\Omega}_i\right)$ for each source i that is representative of that entire source where the biased source will match the target weight windows. For each source, a vector $\widehat{n}_i = \widehat{n}\left(\overrightarrow{r}_i, E_i\right)$ is computed using that point. For the general case of multiple sources, the biased source sampling distribution, the biased source distributions, and the weight windows are computed using

$R_i = \iint q_i\left(\overrightarrow{r}, E\right)\ \phi^{+}\left(\overrightarrow{r}, E\right) dE\ dr$ (estimated response from source i)

$\widehat{p}\left(i\right) = \frac{S_i R_i\ f\left(\widehat{\Omega}_i \bullet \widehat{n}_i\right)}{\sum S_i R_i\ f\left(\widehat{\Omega}_i \bullet \widehat{n}_i\right)}$ (biased sampling of source i)

$$\widehat{q}_i\left(\overrightarrow{r}, E, \widehat{\Omega}\right) = \frac{1}{R_i} q_i\left(\overrightarrow{r}, E\right)\ \phi^{+}\left(\overrightarrow{r}, E\right)\ \frac{1}{2\pi} q_i\left(\widehat{\Omega} \bullet \widehat{d}_i\right) = \widehat{q}_i\left(\overrightarrow{r}, E\right)\ \frac{1}{2\pi} q_i\left(\widehat{\Omega} \bullet \widehat{d}_i\right)$$

$$\overline{w}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) = \frac{\sum S_i R_i\ f\left(\widehat{\Omega}_i \bullet \widehat{n}_i\right)}{S\phi^{+}\left(\overrightarrow{r}, E\right)} \frac{1}{f\left(\widehat{\Omega} \bullet \widehat{n}\right)} = \frac{\sum S_i R_i\ f\left(\widehat{\Omega}_i \bullet \widehat{n}_i\right)}{\sum S_i R_i} \overline{w}\left(\overrightarrow{r}, E\right) \frac{1}{f\left(\widehat{\Omega} \bullet \widehat{n}\right)}$$

4.2.3 Directionally dependent weight windows with directional source biasing

Here it is proposed that the biased source be proportional to both the true source distribution and the approximation of the adjoint angular flux. With a small geometric source, it is also assumed that there is one vector, $\widehat{n}_0 = \widehat{n}\left(\overrightarrow{r}_0, E_0\right)$, evaluated at a specific location and energy, which represents the adjoint current direction over that source. The biased source then looks like

$$\begin{aligned}\widehat{q}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) &= \frac{1}{\mathrm{Rc}} q\left(\overrightarrow{r}, E, \widehat{\Omega}\right)\ \psi^{+}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) \\ &= \frac{1}{\mathrm{Rc}}\left[q\left(\overrightarrow{r}, E\right)\ \frac{1}{2\pi} q\left(\widehat{\Omega} \bullet \widehat{d}_i\right)\right]\ \left[\phi^{+}\left(\overrightarrow{r}, E\right)\ \frac{1}{2\pi}\ f\left(\widehat{\Omega} \bullet \widehat{n}_0\right)\right]\ ,\end{aligned}$$

where the constant Rc is used to make $\widehat{q}$ a pdf. Note that if either the original source directional distribution $q\left(\widehat{\Omega}\right)$ or the adjoint angular flux distribution at the source is isotropic, then $c = \frac{1}{4\pi}$.

For the general case of multiple sources, the biased source sampling distribution, the biased source distributions and the weight windows are

$$R_i = \iint q_i\left(\overrightarrow{r}, E\right)\ \phi^+\left(\overrightarrow{r}, E\right)\text{dE dr}$$

$$c_i = \int \frac{1}{2\pi} q_i\left(\widehat{\Omega} \bullet \widehat{d}_i\right)\ \frac{1}{2\pi} f\left(\widehat{\Omega} \bullet \widehat{n}_i\right) d\widehat{\Omega}$$

$$\widehat{p}\left(i\right) = \frac{S_i R_i c_i}{\sum S_i R_i c_i}$$

$$\widehat{q}_i\left(\overrightarrow{r}, E, \widehat{\Omega}\right) = \left[\frac{1}{R_i}\ q_i\left(\overrightarrow{r}, E\right)\ \phi^+\left(\overrightarrow{r}, E\right)\right]\ \left[\frac{1}{c_i}\ q_i\left(\widehat{\Omega}\right)\ f\left(\widehat{\Omega}\right)\right] = \widehat{q}_i\left(\overrightarrow{r}, E\right)\ \frac{1}{c_i}\ \frac{1}{2\pi} q_i\left(\widehat{\Omega} \bullet \widehat{d}_i\right)\ \frac{1}{2\pi} f\left(\widehat{\Omega} \bullet \widehat{n}_i\right)$$

$$\overline{w}\left(\overrightarrow{r}, E, \widehat{\Omega}\right) = \frac{\sum S_i R_i c_i}{S\phi^+\left(\overrightarrow{r}, E\right)}\ \frac{2\pi}{f\left(\widehat{\Omega} \bullet \widehat{n}\right)} = \frac{\sum S_i R_i c_i}{\sum S_i R_i}\ \overline{w}\left(\overrightarrow{r}, E\right)\ \frac{2\pi}{f\left(\widehat{\Omega} \bullet \widehat{n}\right)}\ .$$

More details on the development of these methods and their application for several problems have been presented [PMEW10][PME12].

4.2.4 Using space/energy/angle CADIS in MAVRIC

The two angular CADIS methods that use the AVATAR-type approximation of adjoint flux are specified in MAVRIC with the "angularBiasing=" keyword in the importanceMap block. Values for this keyword are 1 or 2.

Space/Energy/Angle CADIS without directional biasing (for beam sources) – This method uses one specific location, $\overrightarrow{r}_0$, energy, E_0, and direction, $\widehat{\Omega}_0$, which is the reference direction of the source $\widehat{d}$, where the weight of the biased source matches the weight window.

Space/Energy/Angle CADIS with directional biasing (for general sources) – This method uses one specific energy, E_0, to determine the adjoint current vector $\widehat{n}_0$ and the λ_0 parameter for the biased angular distribution for each source.

With each method, the user must specify at what energy the importance map and the biased sources should be made consistent. The particle type must also be specified. This is done with the keywords "angBiasParType=" (1 for neutron or 2 for photon) and "angBiasEnergy=" (with a value in eV), also in the importanceMap block.

Note that all sources should have a direction $\widehat{d}$ set, using "direction *u v w*" within each source, even if the angular distribution for a given source is isotropic. The direction is used for source biasing and for aligning the weight windows and biased sources. Also note that for either angular biasing method, the Denovo S_N calculation must use a Legendre order greater than 0.

With angular biasing, a mesh angular information (*.mai) file is produced which can be visualized with the MeshFileViewer. This file contains the space/energy-dependent $\lambda\left(\overrightarrow{r}, E\right)$ values and components of the average adjoint current direction $\widehat{n}\left(\overrightarrow{r}, E\right) = \langle n_x, n_y, n_z \rangle$. An existing mesh angular information (*.mai) file can be used in a separate MAVRIC problem by using the "meshAngInfoFile=" keyword in the biasing block.

4.2.5 Example problem

Consider the Ueki shielding problem used as sample problems in the Monaco and MAVRIC manuals. The goal is to calculate the neutron dose on one side of a shield from a partially collimated ^{252}Cf source on the other side of the shield. Both of the angular approaches discussed above can be compared to analog and standard space/energy CADIS calculations. For the analog calculations, no importanceMap block is used. For the other cases, the importance map blocks are shown below.

CADIS	AngularCADIS 1 - without a biased source angular dist.	AngularCADIS 2 - with a biased source angular dist.
read importanceMap adjoint Source	read importanceMap adjoint Source	read importanceMap adjoint Source

Note that the energy at which to tie the importance map to the biased source, 2 MeV, is about the average energy of the source energy distribution. The figure-of-merit (FOM) of the calculation could change as this parameter is varied.

Results, shown in Table 4.1, demonstrate that the two directional approaches improved the FOM for this problem by more than a factor of 2. A larger boost is seen in method 2 where biasing is applied to the source directional distribution. In this case, the biased source distribution was an exponential distribution with a power of 2.45, significantly sampling more source neutrons in the direction of the shield than into the paraffin collimator block.

Note that the space/energy/angle CADIS methods require more memory to hold the importance information. Improvements to the CADIS calculation can also be made with a judicious choice of standard source direction biasing, without an increase in memory requirements. A simple distribution (where $\mu = 0.924$ represents the edge of the cone cutout and $\mu = 0.974$ is the center half of the shield dimension) added that to the source

```
d
i
s
t
r
i
b
u
t
i
o
n 2

a
b
s
c
i
s
s
a
-1
.0      0
.924
.974    1
.0 end

t
r
u
e
p
d
f       0
.962      0
.025
.013    end

b
i
a
s
e
d
p
d
f     0
.500      0
.250   0
.250    end
```

(continues on next page)

(continued from previous page)

```
end
 distribution


s
r
c 1

n
e
u
t
r
o
n
s
s
t
r
e
n
g
t
h=4.05E+07

c
u
b
o
i
d  0
.01 0
.01  0 0  0 0

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1

d
i
r
e
c
t
i
o
n 1
.0 0
.0 0
.0
```

(continues on next page)

(continued from previous page)

```
d
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=2
end
 src
```

results in an FOM improvement of nearly 3 over the standard CADIS without the overhead of the angular CADIS methods.

Table 4.1: Results of the Ueki Shielding Problem (35 cm graphite shield)

Calculation Method	Adj. S_N (min)	MC (min)	dose rate (rem/hr)	relative uncert	MC FOM (/min)
Analog	0.0	152.7	3.998E-03	0.0101	64.7
CADIS	0.2	9.9	3.998E-03	0.0081	1550
Directional CADIS 1, no src bias	0.2	10.3	4.035E-03	0.0054	3390
Directional CADIS 2, with src bias	0.2	10.0	4.012E-03	0.0049	4190
CADIS, standard src dir. bias	0.2	10.0	3.998E-03	0.0047	4550

A series of problems was used to compare the space/energy/angle CADIS to the standard space/energy CADIS. Most of the problems saw an improvement of a factor of about 2 or 3. Some problems did not improve at all, and some photon problems actually performed worse. In that case (a photon litho-density gauge), it could be that the angular approximation for importance, an exponential function in μ, cannot adequately describe the true importance.

Since the space/energy/angle CADIS methods are more difficult to explain (more theory, adjustable parameters set by the user), require more memory than standard CADIS, and may not offer any improvement over standard space/energy CADIS, they have not been made part of the main MAVRIC manual and have been left as an advanced/developing feature. These methods were not removed from the MAVRIC code since they may be helpful to future problems.

4.3 University of Michigan methods for global variance reduction

The use of hybrid deterministic/Monte Carlo methods, particularly for global variance reduction, has been an active area of research by the transport team at the University of Michigan for a long time. One of the first approaches studied was a way to develop Monte Carlo weight window target values that were proportional to deterministically estimated values of the forward flux [CL01]. For global problems using isotropic weight windows, this reference argues that in order to get uniform relative uncertainties in the Monte Carlo calculation, the weight windows should be set such that the number density of Monte Carlo particles, $m\left(\overrightarrow{r}\right)$, is constant. The physical particle density, $n\left(\overrightarrow{r}\right)$, is related by the average weight, $\overline{w}\left(\overrightarrow{r}\right)$, to the Monte Carlo particle density by

$$n\left(\overrightarrow{r}\right) = \overline{w}\left(\overrightarrow{r}\right)\ m\left(\overrightarrow{r}\right)\ .$$

To make $m\left(\overrightarrow{r}\right)$ constant over the geometry, the weight window targets $\overline{w}\left(\overrightarrow{r}\right)$ need to be proportional to the physical particle density. Cooper and Larsen calculate the weight window targets from an estimate of the forward scalar flux $\phi\left(\overrightarrow{r}\right)$ to be

$$\overline{w}\left(\overrightarrow{r}\right) = \frac{\phi\left(\overrightarrow{r}\right)}{\max\left(\phi\left(\overrightarrow{r}\right)\right)}\ .$$

Two approaches have since been developed [BL09], based on what global information the user desires from the simulation: global flux weight windows, for obtaining every energy group at every location, and global response weight windows, for obtaining an energy-integrated response at every spatial location. Both of these methods are designed for calculating the "global solution" – everywhere in the geometry of the problem – with nearly uniform statistics.

Note that none of the University of Michigan methods discussed here included the development of biased sources. These methods have all been extended to include a consistent biased source by ORNL during their implementation in the MAVRIC sequence of SCALE. The methods have also been extended by ORNL for multiple sources.

4.3.1 Weight windows using only forward estimates of flux

Global flux weight windows

This method keeps the Monte Carlo particle distribution uniform in space and energy. Note that this is a space/energy version of the original space-only Cooper's Method. The target weight windows, $\overline{w}\left(\overrightarrow{r}, E\right)$, should be proportional to the estimate of the forward scalar flux, $\phi\left(\overrightarrow{r}, E\right)$.

$$\overline{w}\left(\overrightarrow{r}, E\right) = c\,\phi\left(\overrightarrow{r}, E\right)\ .$$

A biased source distribution, $\widehat{q}\left(\overrightarrow{r}, E\right)$, that is consistent with the target weight windows can be found from the true source distribution, $q\left(\overrightarrow{r}, E\right)$, and the forward flux to be

$$\widehat{q}\left(\overrightarrow{r}, E\right) = \frac{1}{c}\,\frac{q\left(\overrightarrow{r}, E\right)}{\phi\left(\overrightarrow{r}, E\right)}\ ,$$

where the constant c can be determined so that the biased source distribution is a probability distribution function,

$$c = \int_V \int_E \frac{q\left(\overrightarrow{r}, E\right)}{\phi\left(\overrightarrow{r}, E\right)}\ \mathrm{dE}\ d\overrightarrow{r}\ .$$

Thus, using the estimate of forward flux, we can first compute c and then form a consistent set of weight window target values and a biased source distribution.

Global response weight windows

For an energy-integrated response (such as dose) desired at all spatial locations, this method keeps the Monte Carlo particle distribution proportional to the integral of the product of the response function, $\sigma_d\left(\overrightarrow{r}, E\right)$, and the estimate of the forward flux, $\phi\left(\overrightarrow{r}, E\right)$. The energy-integrated response, $D\left(\overrightarrow{r}\right)$, is found from the estimate of the forward flux as

$$D\left(\overrightarrow{r}\right) = \int_E \sigma_d\left(\overrightarrow{r}, E\right)\ \phi\left(\overrightarrow{r}, E\right) DE.$$

The target weight windows, $\overline{w}\left(\overrightarrow{r}, E\right)$, should be

$$\overline{w}\left(\overrightarrow{r}, E\right) = c\ \frac{D\left(\overrightarrow{r}\right)}{\sigma_d\left(\overrightarrow{r}, E\right)}\ .$$

A biased source distribution, $\widehat{q}\left(\overrightarrow{r}, E\right)$, that is consistent with the target weight windows can be found from the true source distribution, $q\left(\overrightarrow{r}, E\right)$, and the forward dose estimate to be

$$\widehat{q}\left(\overrightarrow{r}, E\right) = \frac{1}{c}\ \frac{q\left(\overrightarrow{r}, E\right)\ \sigma_d\left(\overrightarrow{r}, E\right)}{D\left(\overrightarrow{r}\right)}$$

using a proportionality constant of

$$c = \int_V \frac{1}{D\left(\overrightarrow{r}\right)} \int_E q\left(\overrightarrow{r}, E\right)\ \sigma_d\left(\overrightarrow{r}, E\right)\ \text{dE}\ d\overrightarrow{r}\ .$$

Implementation in MAVRIC

The global flux weight windows (GFWW) approach and the global response weight windows (GRWW) are both triggered by specifying an importance map block without any adjoint sources. For the GRWW approach, the response of interest is listed in the importance map block. If none is listed, GFWW is used.

For problems with multiple sources (each with probability distribution function $q_i\left(\overrightarrow{r}, E\right)$ and strength S_i, giving a total source strength of $S = \sum S_i$), the GWW methods require a biased mesh source for each. This was implemented in MAVRIC in a manner similar to the multiple source CADIS routines. Each biased source, $\widehat{q}_i\left(\overrightarrow{r}, E\right)$, is developed as

$$\widehat{q}_i\left(\vec{r}, E\right) = \begin{cases} \frac{1}{c_i}\ \frac{q_i(\vec{r},E)}{\phi(\vec{r},E)} & \text{global flux weight windows} \\ \frac{1}{c_i}\ \frac{q_i(\vec{r},E)\sigma_d(\vec{r},E)}{D(\vec{r})} & \text{global response weight windows} \end{cases}$$

where c_i is a normalization constant. The weight windows are then set to

$$\overline{w}\left(\overrightarrow{r}, E\right) = \begin{cases} \frac{\sum c_i}{\sum S_i}\ \phi\left(\overrightarrow{r}, E\right) & \text{global flux weight windows} \\ \frac{\sum c_i}{\sum S_i}\ \frac{D\left(\overrightarrow{r}\right)}{\sigma_d\left(\overrightarrow{r}, E\right)} & \text{global response weight windows} \end{cases}\ .$$

In the final Monte Carlo, the specific source *i* is sampled with probability $p\left(i\right) = S_i/S$, and then the particle is sampled from the biased mesh source $\widehat{q}_i\left(\overrightarrow{r}, E\right)$. Unlike the CADIS method for multiple sources, there is no way to develop a biased probability distribution for which source to sample without knowing the contribution to the global estimate from each source separately.

For multiple source problems where the expected contribution from each source is very different from the true strengths of those sources, it may be more efficient to run a series of problems with one source each for different amounts of time. The resulting mesh tallies can then be added together using the mesh tally adder (part of the MAVRIC utilities).

4.3.2 Methods using forward and adjoint estimates

Becker [Bec09] proposed three methods for developing weight windows based on both forward and adjoint deterministic solutions. These three methods correspond to the portion of the phase space over which uniform relative uncertainties are desired: a small "detector" region, a region comprising a significant portion of the entire problem, and the global problem. In this discussion, only a brief outline of each method, focusing on its implementation into MAVRIC, will be given.

Source/detector problems

For a small detector of volume $V_D$where we want to optimize the MC calculation of the detector response

$$R = \int_{V_D} \int_0^\infty \sigma\left(\overrightarrow{r}, E\right)\ \phi\left(\overrightarrow{r}, E\right)\text{dE dV}$$

or optimize for the energy dependent flux at the detector, the following is used:

forward flux estimate

$$\phi\left(\overrightarrow{r}, E\right) \tag{4.5}$$

adjoint source for flux

$$q^+\left(\overrightarrow{r}, E\right) = \frac{1}{\phi\left(\overrightarrow{r}, E\right)}$$

or for response

$$q^+\left(\overrightarrow{r}, E\right) = \sigma\left(\overrightarrow{r}, E\right)$$

adjoint flux

$$\phi^+\left(\overrightarrow{r}, E\right)$$

contributon flux

$$\phi^c\left(\overrightarrow{r}, E\right) = \phi\left(\overrightarrow{r}, E\right)\ \phi^+\left(\overrightarrow{r}, E\right)$$

normalization constant

$$C_{\text{norm}} = \frac{V_D}{\int_{V_D} \int_0^\infty \phi^c\left(\overrightarrow{r}, E\right) dE\ dV}$$

space-only contributon flux

$$\widetilde{\phi}^c\left(\overrightarrow{r}\right) = C_{\text{norm}} \int_0^\infty \phi^c\left(\overrightarrow{r}, E\right) dE$$

spatial parameter

$$\alpha\left(\overrightarrow{r}\right) = \left[1 + exp\left(\frac{\widetilde{\phi}^c_{\max \in V_D}}{\widetilde{\phi}^c\left(\overrightarrow{r}\right)} - \frac{\widetilde{\phi}^c\left(\overrightarrow{r}\right)}{\widetilde{\phi}^c_{\max \in V_D}}\right)\right]^{-1}$$

spatial parameter

$$B\left(\overrightarrow{r}\right) = \alpha\left(\overrightarrow{r}\right)\widetilde{\phi}^{c}\left(\overrightarrow{r}\right) + 1 - \alpha\left(\overrightarrow{r}\right)$$

weight windows

$$\overline{w}\left(\overrightarrow{r}, E\right) = \frac{B\left(\overrightarrow{r}\right)}{\phi^{+}\left(\overrightarrow{r}, E\right)} \tag{4.6}$$

Source-region problems

For a detector of volume V_D and surface area A_D (smaller than the entire problem) where we want to optimize the MC calculation of the detector response

$$R\left(\overrightarrow{r}\right) = \int_{0}^{\infty} \sigma\left(\overrightarrow{r}, E\right)\ \phi\left(\overrightarrow{r}, E\right) dE \qquad \overrightarrow{r} \in V_D$$

or optimize for the energy dependent flux in the region, the following is used:

forward flux estimate

$$\phi\left(\overrightarrow{r}, E\right) \tag{4.7}$$

adjoint source for flux

$$q^{+}\left(\overrightarrow{r}, E\right) = \frac{1}{\phi\left(\overrightarrow{r}, E\right)}$$

adjoint source for response

$$q^{+}\left(\overrightarrow{r}, E\right) = \frac{\sigma\left(\overrightarrow{r}, E\right)}{\int_{0}^{\infty} \sigma\left(\overrightarrow{r}, E\right)\ \phi\left(\overrightarrow{r}, E\right) dE}$$

adjoint flux estimate

$$\phi^{+}\left(\overrightarrow{r}, E\right)$$

contributon flux

$$\phi^{c}\left(\overrightarrow{r}, E\right) = \phi\left(\overrightarrow{r}, E\right)\ \phi^{+}\left(\overrightarrow{r}, E\right)$$

normalization constant

$$C_{\text{norm}} = \frac{A_D}{\int_{A_D} \int_{0}^{\infty} \phi^{c}\left(\overrightarrow{r}, E\right) dE\ dA}$$

space-only contributon flux

$$\widetilde{\phi}^{c}\left(\overrightarrow{r}\right) = C_{\text{norm}} \int_{0}^{\infty} \phi^{c}\left(\overrightarrow{r}, E\right) dE$$

spatial parameter

$$\alpha\left(\overrightarrow{r}\right) = \left[1 + exp\left(\frac{\widetilde{\phi}^{c}_{\max \in V_D}}{\widetilde{\phi}^{c}\left(\overrightarrow{r}\right)} - \frac{\widetilde{\phi}^{c}\left(\overrightarrow{r}\right)}{\widetilde{\phi}^{c}_{\max \in V_D}}\right)\right]^{-1}$$

spatial parameter

$$B\left(\vec{r}\right) = \begin{cases} \tilde{\phi}^{c}\left(\vec{r}\right) & \vec{r} \in V_D \\ \alpha\left(\vec{r}\right)\tilde{\phi}^{c}\left(\vec{r}\right) + 1 - \alpha\left(\vec{r}\right) & \text{otherwise} \end{cases} \tag{4.8}$$

weight windows

$$\overline{w}\left(\overrightarrow{r}, E\right) = \frac{B\left(\overrightarrow{r}\right)}{\phi^{+}\left(\overrightarrow{r}, E\right)}$$

Note that A_D does not include surfaces of V_D which are on the boundary of the problem.

Global response problem

For optimizing the Monte Carlo calculation of a detector response everywhere in phase space

$$R(\overrightarrow{r}) = \int_0^{\infty} \sigma\left(\overrightarrow{r}, E\right)\ \phi\left(\overrightarrow{r}, E\right)\text{dE}$$

or optimizing for the energy-dependent flux everywhere, the following is used:

forward flux estimate

$$\phi\left(\overrightarrow{r}, E\right) \tag{4.9}$$

adjoint source for flux

$$q^{+}\left(\overrightarrow{r}, E\right) = \frac{1}{\phi\left(\overrightarrow{r}, E\right)}$$

adjoint source for response

$$q^{+}\left(\overrightarrow{r}, E\right) = \frac{\sigma\left(\overrightarrow{r}, E\right)}{\int_0^{\infty} \sigma\left(\overrightarrow{r}, E\right)\ \phi\left(\overrightarrow{r}, E\right)dE}$$

adjoint flux estimate

$$\phi^{+}\left(\overrightarrow{r}, E\right)$$

contributon flux

$$\phi^{c}\left(\overrightarrow{r}, E\right) = \phi\left(\overrightarrow{r}, E\right)\ \phi^{+}\left(\overrightarrow{r}, E\right)$$

space-only contributon flux

$$\phi^{c}\left(\overrightarrow{r}\right) = \int_0^{\infty} \phi^{c}\left(\overrightarrow{r}, E\right)dE$$

spatial parameter

$$B\left(\overrightarrow{r}\right) = \phi^{c}\left(\overrightarrow{r}\right)$$

weight windows

$$\overline{w}\left(\overrightarrow{r}, E\right) = \frac{B\left(\overrightarrow{r}\right)}{\phi^{+}\left(\overrightarrow{r}, E\right)}$$

4.3.3 Implementation in MAVRIC

Like CADIS and FW-CADIS, the Denovo S_N code is used to calculate the forward flux estimate, $\phi\left(\overrightarrow{r}, E\right)$, and the estimate of the adjoint flux, $\phi^{+}\left(\overrightarrow{r}, E\right)$, for all of the Michigan weight window methods.

None of the above discussions of the University of Michigan methods include information on how the weight window target values were adjusted to match the source sampling. When implemented into MAVRIC, each of the above problem types will compute a biased source, $\widehat{q}\left(\overrightarrow{r}, E\right)$, along with the target weight, $\overline{w}\left(\overrightarrow{r}, E\right)$, that are produced. For a problem with a single source of strength S and distribution $q\left(\overrightarrow{r}, E\right)$, the biased source distribution $\widehat{q}\left(\overrightarrow{r}, E\right)$ is found by using

$$\widehat{q}\left(\overrightarrow{r}, E\right) = \frac{q\left(\overrightarrow{r}, E\right)}{\overline{w}\left(\overrightarrow{r}, E\right)} \ .$$

The weight windows are multiplied by a factor of R/S, where R is defined as

$$R = \iint \widehat{q}\left(\overrightarrow{r}, E\right)\phi^{+}\left(\overrightarrow{r}, E\right) \ dE \ dV.$$

Sampled source particles will then be born with a weight that matches the weight window of the phase space where they are born.

For multiple sources, each with strength S_i and distribution $q_i\left(\overrightarrow{r}, E\right)$, each biased source distribution $\widehat{q}_i\left(\overrightarrow{r}, E\right)$ is found by using

$$\widehat{q}_i\left(\overrightarrow{r}, E\right) = \frac{q_i\left(\overrightarrow{r}, E\right)}{\overline{w}\left(\overrightarrow{r}, E\right)}$$

and the response from each source being

$$R_i = \iint \widehat{q}_i\left(\overrightarrow{r}, E\right) dE \ dV \ .$$

The individual sources are sampled with a biased probability of $\widehat{p}\left(i\right) = \ R_i / \sum R_i$. The weight windows are then multiplied by a factor of

$$\frac{\sum_i R_i}{\sum_i S_i}$$

to match the source birth weights.

To use one of the Becker methods in MAVRIC, the keyword "beckerMethod=" is used with values of 1, 2, or 3 for the source/detector, source/region, or global method. Adjoint sources are described just like standard MAVRIC CADIS and FW-CADIS problems. To switch between optimizing flux in every group or optimizing a response, the keywords "fluxWeighting" and "respWeighting" are used. Just like FW-CADIS, the response listed in each adjoint source is the response that is optimized. Note that even when starting a calculation with known forward and adjoint flux files, the adjoint source(s) still need to be listed since they are used in the final normalization of the weight windows.

Example problems

The first Becker method (source/detector) is demonstrated using the Ueki shielding problem (used as sample problems in the Monaco and MAVRIC manuals and above in the space/energy/angle CADIS example). The goal is to calculate the neutron dose on one side of a shield from a partially collimated ^{252}Cf source on the other side of the shield. For the analog calculations, no importanceMap block is used. For the other cases, the importance map blocks are shown below.

CADIS	Becker 1-fluxoptimization	Becker 2-responseoptimization
read importanceMap adjointSource 1 locationID=1	read importanceMap adjointSource 1 locationID=1	read importanceMap adjointSource 1 locationID=1
response	response	response

The results are shown in Table 4.2. The Becker response-optimized source/detector method, which requires two deterministic estimates, does slightly better for this problem than standard CADIS, which only requires one deterministic estimate.

Table 4.2: Results of the Ueki Shielding Problem (35 cm graphite shield)

Calculation method	For. S_N	Adj. S_N	MC	dose rate (rem/hr)	relative uncert	MC FOM (/min)
Analog	0.0	0.0	152.7	3.998E-03	0.0101	6.47
CADIS	0.0	0.2	9.9	3.988E-03	0.0081	1550
Becker, source/detector flux	0.2	0.2	9.9	4.027E-03	0.099	1040
Becker, source/detector resp	0.2	0.2	10.1	4.025E-03	0.0075	1760

A global problem

For an example of a global problem, consider a two-room block building with a criticality accident in one room. The objective is to find the photon dose everywhere in order to see the locations where criticality alarms would trigger. The building is 12 meters long, 6 meters wide, and 3 meters tall. A comparison will be made between an analog calculation, an FW-CADIS calculation (using response weighting), GRWW, Becker's source/region method (response optimization), and Becker's global method (response optimization). The MAVRIC importance map block of each calculation is as follows.

FW-CADIS	GRWW	Beckersource/region	Becker-global
read importanceMap gridGeometryID=1 adjointSource 1 bounding	read importanceMap gridGeometryID=1 responseID=6 end importanceMap	read importanceMap gridGeometryID=1 adjointSource 1 bounding	read importanceMap gridGeometryID=1 adjointSource 1 bounding

Note that Becker's source/region method is designed for regions smaller than the entire problem, so this is not a fair comparison, just a demonstration on how to use it in MAVRIC. The bounding box of the adjoint source in this case is set slightly smaller than the extent of the entire problem.

Results for the photon dose and its relative uncertainty using the five different methods of calculation are shown in Fig. 4.3. Information on the distribution of relative uncertainties is shown in Fig. 4.4 and listed in Table 4.3.

A more detailed comparison of the different hybrid methods for representative shielding problems can be found in [Pep13].

Table 4.3: Comparison of the five different methods

Calculation method	Forward S_N (min)	Adjoint S_N (min)	Monte Carlo (min)	fraction of voxels with relative uncertainties less than 5%	fraction of voxels with relative uncertainties less than 10%	fraction of voxels with relative uncertainties less than 15%
Analog			20.1	0.583	0.857	0.973
Analog, long			308.1	0.996	1.000	1.000
FW-CADIS, response weighting	3.5	3.4	20.3	0.946	1.000	1.000
GRWW	4.0		20.2	0.005	0.180	0.387
Becker, source/region	4.0	3.6	19.0	0.016	0.350	0.800
Becker, global response	4.2	4.4	20.4	0.016	0.358	0.832

4.3.4 Other special options for the importance map block input

In MAVRIC, the above methods have been extended to use biased sources. To turn off the use of a biased source, use the keyword "selfNormalize". For forward flux–based methods, this will scale the target weights in the importance map so that the largest value is 1, which typically is at the source location. To use the forward-based Michigan methods (Cooper, GFWW, GRWW) or the van Wijk [VWVdEH11] methods as they were presented (without the MAVRIC biased source), use this keyword.

Use the keyword "spaceOnly=n" to create an importance map that contains one energy group over the entire range of energy. Use a value of 1 for neutron problems or a value of 2 for photon problems. This option is not designed for coupled problems. Both of the methods that van Wijk presents use importance maps that are space only.

Use the keyword "forwardParam=p" to allow the target weights to be proportional to the forward estimate (using Denovo) of flux raised to any power p.

$$\overline{w}\left(\overrightarrow{r}\right) = \frac{\phi^p\left(\overrightarrow{r}\right)}{\max\left(\phi^p\left(\overrightarrow{r}\right)\right)} \ .$$

For Cooper's method or van Wijk's first method, $p = 1$, which is the default if "forwardParam" is not specified. For van Wijk's second method, based on the relative error estimate Re $\left(\overrightarrow{r}\right) \propto \frac{1}{\sqrt{\phi\left(\overrightarrow{r}\right)}}$, set this parameter to $p = 0.5$. Note that with a power less than 1, the weight window targets will span a smaller range than the expected Monte Carlo flux values. Particles may be rouletted before they reach the lowest flux areas of the problem.

When applying FW-CADIS for a semi-global problem, the adjoint source should cover the area where the lowest uncertainties are desired. Sometimes the area where this is desired is not a fixed geometric area but instead an area that has a final answer of a certain range. For example, when finding dose rate maps, the user may only be interested

Fig. 4.3: Mesh tally results for the photon dose over the entire building use five different methods.

Fig. 4.4: The fraction of mesh tally voxels with less than a given amount of relative uncertainty for the five different methods.

in getting low uncertainties for areas below the dose limit – areas above the dose limit may not matter as much since people will not be allowed in those areas. Another example may be that the dose map should be optimized in those areas above the background dose rate, since dose rates below that are of no concern. To allow the adjoint source area to be tailored in this way, the keywords "minForwardValue=" and/or "maxForwardValue="can be used. Default values are 0 and 10^{100}, respectively. For flux weighting, only the voxels within the adjoint source bounding box and containing a forward flux estimate between the min and max are included as adjoint sources.

A comparison [Pep13] of FW-CADIS to the University of Michigan methods and the Van Wijk methods showed that FW-CADIS performs better and is more straightforward to use than the other methods. These other methods were added to SCALE so that a fair comparison could be made and have been left in the code base for academic use in case some types of problems could benefit from them.

4.4 Using MAVRIC to run fixed-source Denovo calculations

The MAVRIC sequence of SCALE can be used to run the new discrete-ordinates code Denovo [ESSC10] The sequence is designed to use Denovo to compute an importance map for the Monte Carlo code Monaco but can be stopped without starting the final Monaco calculation. The full version of Denovo has a python-based user interface where the user must construct the geometry, source, and cross sections on their own. MAVRIC provides an easy interface to run the serial-only version of Denovo within SCALE (called 'xkba'). Denovo inputs made using MAVRIC can also be imported into the python interface for the HPC version of Denovo.

To create Denovo inputs or run Denovo using MAVRIC, input the composition, geometry (including arrays if needed), definitions (grid geometry and response information), and sources block as if an actual full MAVRIC case were being run. The sequence should then be started with a `parm=xxx` flag to indicate to MAVRIC to stop after making Denovo inputs or running Denovo.

parm=	MAVRIC stops after
Forward Calculations	
forinp	Making cross sections and Denovo input
forward	Running Denovo
Adjoint Calculations	
adjinp	Making cross sections and Denovo input
adjoint	Running Denovo

For forward Denovo simulations, the importance map block should contain which grid geometry to use and any of the optional Denovo parameters:

For forward Denovo simulations, the importance map block should contain which grid geometry to use and any of the optional Denovo parameters:

```
read
 importanceMap

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=7
end
 importanceMap
```

For adjoint Denovo calculations, the importance map block should contain which grid geometry to use, one or more adjoint sources, and any of the optional Denovo parameters:

```
read
 importanceMap

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=7
```

(continues on next page)

(continued from previous page)

```
a
d
j
o
i
n
t
S
o
u
r
c
e 1

l
o
c
a
t
i
o
n
I
D
=1

r
e
s
p
o
n
s
e
I
D
=5
    end
 adjointSource
end
 importanceMap
```

For either forward or adjoint, the following files will be produced and should be copied out of the SCALE temporary directory back to your home area:

ft02f001	the AMPX mixed working library cross section file
xkba_b.inp	binary input file for Denovo
*.dff	Denovo flux file (binary) - scalar fluxes

The scalar flux file is automatically copied back to the home area when SCALE completes. The others can be copied back if desired using a shell command at the end of the MAVRIC input file (windows example shown below):

```
=shell

c
```

(continues on next page)

```
o
p
y
f
t02
f001
%
```

(continued from previous page)

```
c
o
p
y
x
k
b
a
_
b
.
i
n
p
%
{
R
T
N
D
I
R
}
%
/
d
e
n
o
v
o
.
d
s
i
end
```

The xkba_b.inp file and the *.dff file can both be viewed with the Java utility, Mesh File Viewer, that is shipped with SCALE. The xkba_b.inp file shows the Denovo source distribution (space and energy), and the *.dff shows the final computed scalar fluxes. The binary Denovo input file should be renamed with an extension of *.dsi (Denovo simple input) so that the viewer can properly interpret the data.

4.4.1 Optional Denovo parameters

The default values for various calculational parameters and settings used by Denovo for the MAVRIC sequence should cover most applications. These settings can be changed by the interested user in the importance map block. The two most basic parameters are the quadrature set used for the discrete ordinates and the order of the Legendre polynomials used in describing the angular scattering. The default quadrature order that MAVRIC uses is S_8, and for the order of Legendre polynomials, the default is P_3 (or the maximum number of coefficients contained in the cross section library, if less than 3). S_8/P_3 should be a good choice for many applications, but the user is free to changes these. For complex ducts or transport over large distance at small angles, S_{12} may be required. S_4/P_1 would be useful in doing a very cursory run just to check if the problem was input correctly. Other parameters that can be set by the user in the importance map block for Denovo calculations are listed in Table 4.4.

Table 4.4: Optional Denovo parameters for the MAVRIC Importance Map Block

block	keyword	type	length	default	required	restrictions/comments
importanceMap						
Optional Denovo S_N code parameters						
	discretization=	integer		4	no	0-diamond-difference, 1-diamond-difference with flux fix-up:lin0, 2-theta-weighted diamond-difference, 3-linear-discontinuous finite element, 4-step characteristics, 5-trilinear discontinuous finite elem
	quadType=	integer		0	no	0-level symmetric, 1-Gauss-Legendre product, 2-QR
	legendre=	integer		3*	no	P_L, L=highest Legendre polynomial, L=0,1,2,3,… *default is to use min(the highest available in the data,3)
	tportcorrection=	integer		1*	no	transport correction: 0-none, 1-diagonal, 2-Cesaro *For P_2 or higher, the default is 2 (Cesaro)
	upScatter=	integer		0	no	upscatter iterations: 0-none, 1-yes, 2-ignore
	xblocks=	integer		1	no	parallel stuff
	yblocks=	integer		1	no	parallel stuff
	zblocks=	integer		1	no	parallel stuff
	numSets=	integer		1	no	?
	partUpscatter=	integer		1	no	partition upscatter (0-no, 1-yes)
	quadrature=	integer		8	no	level symmetric S_N quadrature, N=2, 4, 6, 8, 10, 12, 14, 16
	polarsPerOct=	integer		0	no	Gauss-Legendre product quadrature or QR
	azimuthsPerOct=	integer		0	no	Gauss-Legendre product quadrature or QR
	maxIters=	integer		20	no	maximum number of iterations
	diagnostics=	integer		0	no	0-no diganostics, 1-all diagnostics
	output=	integer		0	no	0-no ouput, 1-all output
	krylovSpaceSize=	integer		10	no	size in memory for Krylov space
	tolerance=	double		1.E-03	no	tolerance used in convergence test
	krylovType=	integer		0	no	0-GMRES, 1-BiCGStab
	eigenSolver=	integer		0	no	0-power iteration, 1-Arnoldi, 2-shifted inverse
	multiGSolover=	integer		0	no	0-Gauss-Seidel, 1-Krylov
	withinGSolver=	integer		0	no	0-Krylov, 1-residual Krylov, 2-source iteration
	mgSettings=	integer		1	no	0-user supplied, 1-automatic
	upGroupSolver=	integer		0	no	0-same as within-group solver, 1-Krylov, 2-residual Krylov, 3-source iteration, 4-single source iteration
	acceleration=	integer		0	no	0-none, 1-two grid
	maxItersMG=	integer		20	no	maximum number of iterations
	toleranceMG=	double		0.001	no	tolerance used in convergence test
end importanceMap						

In problems with small sources or media that are not highly scattering, discrete ordinates can suffer from "ray effects"—where artifacts of the quadrature directions can be seen in the computed fluxes. To help alleviate the ray effects problem, Denovo has a first-collision capability. This computes the amount of uncollided flux in each mesh cell from a point source. These uncollided fluxes are then used as a distributed source in the main discrete-ordinates solution. At the end of the main calculation, the uncollided fluxes are added to the fluxes computed with the first-collision source, forming the total flux. While this helps reduce ray effects in many problems, the first-collision capability can take a long time to compute on a mesh with many cells or for many point sources.

The macromaterials option ("mmTolerance=") can be used to better represent the geometry in Denovo. Refer to the main MAVRIC manual for details on macromaterials.

4.4.2 Forward source preparations

The user-entered source description is converted to a mesh-based source for Denovo. To create the mesh source, MAVRIC determines if the defined source exists within each cell. This is done by dividing each mesh cell into $n \times n \times n$ subcells (from the keyword "subCells=n" in the importance map block with a default of n=2) and testing each subcell center. For every subcell center that is a valid source position (within the spatial solid and meets optional unit, region, or mixture requirements), an amount of source proportional to the subcell volume is assigned to the mesh cell. The keyword "subCells=" can be used to better refine how much source is computed for the mesh cells at the boundary of a curved source region. Of course, more subcell testing takes more time.

The above process may miss small sources or degenerate sources (surfaces, lines, points) that do not lie on the tested subcell centers. If none of the mesh cells contain any source after the subcell method, then random sampling of the source is used. A number of source positions are sampled from the source (set by the "sourceTrials=" keyword, default of 1000000) and then placed into the proper mesh cell. If this method is used, the resulting Denovo input file should be visualized to ensure that the statistical nature of the source trials method does not unduly influence the overall mesh source.

For forward calculations, if the number of mesh cells containing the true source is less than 10, then MAVRIC will convert these source voxels to point sources, to allow Denovo to use its first-collision capability to help reduce ray effects. The user can easily override the MAVRIC defaults—to force the calculation of a first-collision source no matter how many voxels contain source—by using the keyword "firstCollision." To prevent the calculation of a first-collision source, the keyword "noFirstCollision" can be used.

For coupled problems, there are two ways to make Denovo compute photon fluxes from a neutron source: 1) include a tally using a photon response or 2) manually specify the "startGroup=" and the "endGroup=" to cover the particles/energy groups that are desired in the final Denovo output.

4.4.3 Adjoint source preparation

For adjoint calculations, adjoint sources that use point locations will use the Denovo first-collision capability. Volumetric adjoint sources (that use a boundingBox) will be treated without the first-collision capability. The keywords "firstCollision" and "noFirstCollision" will be ignored by MAVRIC for adjoint calculations.

Note that for an adjoint Denovo calculation, the MAVRIC input must still list a forward source. Otherwise, the sequence will report an error and stop. The forward source is not used for an adjoint Denovo calculation, but it must be present to make a legal MAVRIC input. For a coupled problem using an adjoint photon source, using a neutron forward source will make Denovo compute both photon and neutron adjoint fluxes. If the forward source(s) and adjoint source(s) are all photon, then only photon adjoint fluxes will be computed. The keywords "startGroup=" and "endGroup=" can also be used to manually set the particles/energy groups that are desired in the final Denovo output.

4.4.4 Other notes

Denovo (in SCALE 6) is a fixed-source S_N solver and cannot model multiplying media. Neither forward nor adjoint neutron calculations from Denovo will be accurate when neutron multiplication is a major source component. If neutron multiplication is not turned off in the parameters block of the MAVRIC input (using keyword "noFissions"), a warning will be generated to remind the user of this limitation.

By default, MAVRIC instructs Denovo not to perform outer iterations for neutron problems if the cross-section library contains upscatter groups. This is because the time required to calculate the fluxes using upscatter can be significantly longer than without. For problems where thermal neutrons are an important part of the transport or tallies, the user should specify the keyword "upScatter=1" in the importance map block. This will instruct Denovo to perform the outer iterations for the upscatter groups, giving more accurate results but taking a longer time.

4.4.5 MAVRIC utilities for Denovo

Denovo simply calculates scalar fluxes for every mesh cell and energy group – it does not compute responses based on those fluxes. Several utilities have been added to the collection of MAVRIC utilities in order to allow the user to further process Denovo scalar flux results. The full details and input descriptions for these utilities can be found in the MAVRIC Utilities description in Appendix B.

dff2dso	Convert a Denovo flux file into a Denovo spatial output file.
dff2mai	Convert a Denovo flux file into a mesh angular information file.
dff2mim	Invert a Denovo flux file and store as a mesh importance map.
dff2msl	Convert a Denovo flux file into a mesh source lite.
dffBinOp	Binary operation of Denovo flux files: sum, difference, product, and ratio.
dffDisp	Display the basics of a Denovo flux file.
dffFilter	Perform various filters on a Denovo flux file.
dffFix	Fix the zero and negative values in a Denovo flux file.
dffInt	Integrate a single particle type from a Denovo flux file.
dffInv	Invert the values in a Denovo flux file.
dffMult	Multiply a Denovo flux file by a constant factor.
dffPull	Pull fluxes from certain voxels out of a Denovo flux file.
dffResp	Apply a response function to scalar fluxes in a Denovo flux file.
dffSplit	Split off a single particle type from a Denovo flux file.

There are also two utility programs that look at the Denovo simple input file (binary) that MAVRIC creates. In the SCALE temporary directory, the file is called xkba_b.inp. In order to display in the MeshFileViewer, Denovo simple input files need to be renamed with a *.dsi extension. The utilities are as follows.

dsi2asc	Convert a Denovo simple input (*.dsi) from binary to ASCII (so the user can see every detail).
dsiDisp	Display the basics of a Denovo simple input file.

4.4.6 Example problem

Forward

As an example, consider a simulation based on the Ueki shielding experiments (see Monaco manual). A ^{252}Cf neutron source was placed in the center of a 50 cm cube of paraffin which had a 45° cone cut-out. The goal is to calculate the neutron dose at a detector 110 cm from the source.

The input file (`denovo1.inp`) needs the compositions of the paraffin and graphite

```
read
 composition

p
a
r
a
(
h2
o
)    3          1
.0 293
.0 end
```

(continues on next page)

(continued from previous page)

```
c
a
r
b
o
n       4
d
e
n
=1
.7 1
.0 293
.0 end
end
 composition
```

then the geometry

```
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

c
u
b
o
i
d  1   25
.0
-25
.0  25
.0
-25
.0   25
.0
-25
.0

c
o
n
e    2  10
.35948  25
.01   0
.0 0
.0
```

(continues on next page)

```
r
o
t
a
t
e
a1
```

(continued from previous page)

```
c
u
b
o
i
d  3   90
.0  70
.0  40
.0
-40
.0   40
.0
-40
.0

c
u
b
o
i
d 99  120
.0
-30
.0  50
.0
-50
.0   50
.0
-50
.0

m
e
d
i
a 3 1  1
-2

m
e
d
i
a 0 1  2

m
e
d
i
a 4 1  3

m
e
d
i
a 0 1  99
-1
-2
-3
```

(continues on next page)

(continued from previous page)

```
b
o
u
n
d
a
r
y 99
end
 geometry
```

then the position of the detector, the response of the detector and the mesh to use for Denovo

```
read
 definitions

l
o
c
a
t
i
o
n 1

p
o
s
i
t
i
o
n 110 0 0
    end
 location

r
e
s
p
o
n
s
e 5

t
i
t
l
e
="ANSI standard (1977) neutron flux-to-dose-rate factors"

s
p
e
c
i
a
l
p
o
s
e
```

(continues on next page)

(continued from previous page)

```
    end
 response

d
i
s
t
r
i
b
u
t
i
o
n 1

t
i
t
l
e
="Cf-252 neutrons, Watt spectrum a=1.025 MeV and b=2.926/MeV"

s
p
e
c
i
a
l
="wattSpectrum"

p
a
r
a
m
e
t
e
r
s 1
.025 2
.926 end
    end
 distribution

g
r
i
d
G
e
o
m
e
t
r
y 7
```

(continues on next page)

(continued from previous page)

```
x
L
i
n
e
a
r 4
-25
-5

x
L
i
n
e
a
r 15
-5 25

x
L
i
n
e
a
r  9 25 70

x
L
i
n
e
a
r  8 70 90

x
p
l
a
n
e
s
-30 95 100 105 109 111 115 120  end


y
p
l
a
n
e
s
-50
-40 40 50 end

y
L
i
n
e
a
r  5
-40
```

(continues on next page)

(continued from previous page)

```
y
L
i
n
e
a
r 15
-15 15

y
L
i
n
e
a
r  5  15 40


z
p
l
a
n
e
s
-50
-40 40 50 end

z
L
i
n
e
a
r  5
-40
-15

z
L
i
n
e
a
r 15
-15 15

z
L
i
n
e
a
r  5  15 40
    end
 gridGeometry
```

(continues on next page)

(continued from previous page)

```
end
 definitions
```

the description of the true source

```
read
 sources

s
r
c 1

n
e
u
t
r
o
n
s
s
t
r
e
n
g
t
h=4.05E+07

c
u
b
o
i
d  0
.01 0
.01  0 0  0 0

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources
```

(continues on next page)

(continued from previous page)

and finally the importance map block to trigger the Denovo calculation

```
read
 importanceMap

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=7

m
m
T
o
l
e
r
a
n
c
e
=0
.001
end
 importanceMap
```

An optional shell command can be used to retrieve the cross section file and the Denovo input file (linux example shown below)

```
=shell

c
p
f
t02
f001
$
{
R
T
N
D
I
R
}
/
d
n
o
v
o1
```

(continues on next page)

(continued from previous page)

```
c
p
x
k
b
a
_
b
.
i
n
p
$
{
R
T
N
D
I
R
}
/
d
e
n
o
v
o1
.
x
k
b
a
.
d
s
i
end
```

The `denovo1.xkba.dsi` file (the Denovo simple input) contains both the source and mesh geometry that MAVRIC prepared for Denovo, as shown in Fig. 4.5.

The result of the Denovo-only MAVRIC calculation is a file, `denovo1.forward.dff`, containing the scalar fluxes for each energy group. The Mesh File Viewer can be used to display each group or the total scalar flux, which is shown in Fig. 4.6.

The MAVRIC utilities can be used to further process the Denovo flux into a detector response. The fluxes at the location of the detector need to be multiplied by the photon flux-to-dose conversion factors (the response function) and then summed. This is can be done in the same input file using

Fig. 4.5: Forward Denovo source (left) and mesh geometry (right).

Fig. 4.6: Total forward fluxes.

```
=dffResp
"denovo1.forward.dff"
1
27
1.6151395E-04
1.4451494E-04
1.2703618E-04
1.2810882E-04
1.2983654E-04
1.0343020E-04
5.2655141E-05
1.2860853E-05
3.7358122E-06
3.7197628E-06
4.0085556E-06
4.2945048E-06
4.4731187E-06
4.5656334E-06
4.5597271E-06
4.5209654E-06
4.4872718E-06
4.4659614E-06
4.4342228E-06
4.3315831E-06
4.2027596E-06
4.0974155E-06
3.8398102E-06
3.6748431E-06
3.6748440E-06
3.6748431E-06
3.6748447E-06
"denovo1.doses.dff"
end
```

```
=dffInt
" denovo1.doses.dff"
1
" denovo1.total.dff"
end


=dffPull
" denovo1.total.dff"
1
110
.0 0
.0 0
.0
0
"denovo1.detectorDose.txt"
end
```

and results in a neutron dose rate of 5.426×10^{-3} rem/hr, calculated in about 2 minutes. Other combinations of the MAVRIC utilities can be used to simply "pull" out the fluxes from the detector location and then use a spreadsheet to compute the dose rate. With upscatter on, the result is 5.424×10^{-3} rem/hr, showing that upscatter does not contribute to dose rate at the detector. Note that with upscatter on, the Denovo calculation required 81 minutes.

Adjoint

For the same calculation of neutron dose as above, a Denovo adjoint calculation can be performed. The input file (`denovo2.inp`) has the same composition, geometry, definitions, and source blocks as the forward example. The adjoint input importance map block contains a description of the adjoint source

```
read
 importanceMap

a
d
j
o
i
n
t
s
o
u
r
c
e 1
```

(continues on next page)

(continued from previous page)

```
l
o
c
a
t
i
o
n
I
D
=1

r
e
s
p
o
n
s
e
I
D
=5
    end
 adjointSource

g
r
i
d
G
e
o
m
e
t
r
y
I
D
=7

m
m
T
o
l
e
r
a
n
c
e
=0
.001
end
 importanceMap
```

(continues on next page)

(continued from previous page)

The result of this Denovo-only MAVRIC calculation is a file, `denovo2.adjoint.dff`, containing the scalar adjoint fluxes for each energy group, as shown in Fig. 4.7.

Fig. 4.7: Total adjoint fluxes.

As with the forward fluxes, the MAVRIC utilities can be used to further process the Denovo adjoint fluxes into a detector response. The adjoint fluxes at the location of the forward source need to be multiplied by the source distribution and strength and then summed. This is can be done using

```
=dffResp
"denovo2.adjoint.dff"
1
27
3.365455E-02
2.398546E-01
2.398289E-01
1.085244E-01
1.527957E-01
1.463752E-01
6.669337E-02
1.164470E-02
5.713197E-04
5.240384E-05
4.470401E-06
2.956226E-07
4.160008E-08
1.011605E-08
9.667897E-10
3.579175E-10
9.880883E-11
6.634570E-11
9.742191E-11
1.538334E-10
2.777230E-11
2.690255E-11
2.572180E-11
7.001169E-12
2.049478E-12
1.437105E-12
3.424200E-13
"denovo2.doses.dff"
end
```

```
=dffMult
" denovo2.doses.dff"
4.05E+07
" denovo2.doses.dff"
end


=dffInt
" denovo2.doses.dff"
1
" denovo2.total.dff"
end


=dffPull
" denovo2.total.dff"
1
0
.0 0
.0 0
.0
0
"denovo2.detectorDose.txt"
end
```

and results in a neutron dose rate of 5.463×10^{-3} rem/hr.

The results of the example problems above used a fairly coarse mesh (44×27×27) and the default values of S_8 and P_3. Run times were 2 minutes for the forward case and 2.5 minutes for the adjoint. With a finer mesh, larger quadrature order and larger numbers of Legendre moments for the scattering representation, the values calculated using Denovo should converge towards the Monte Carlo solution of 1.494×10^{-2} rem/hr $\pm$ 1.2%.

CHAPTER

FIVE

MONACO: A FIXED-SOURCE MONTE CARLO TRANSPORT CODE FOR SHIELDING APPLICATIONS

D. E. Peplow and C. Celik

Monaco is a general-purpose, fixed-source, Monte Carlo shielding code for the SCALE package. It is a functional module that uses either AMPX cross sections or continuous energy libraries to calculate neutron and photon fluxes and responses to specific geometry regions, to point detectors and to mesh tallies. Basic multigroup transport methods are inherited from Monaco's predecessor, MORSE. Continuous energy physics has been incorporated into the code with a new physics package that uses the same CE data as CE-KENO-VI, with extensions for simulating photons. Variance reduction capabilities include source biasing and weight windows, either by geometry region or by using a mesh-based importance map. User input includes the cross section file unit number; the geometry description using the SCALE General Geometry Package; source description as a function of position, energy, and direction; tally descriptions (fluxes in which regions, at what point detectors, or over what mesh grids); and response functions (functions of energy). Output consists of tables detailing the region and point detector fluxes (and their responses), as well as files for mesh tallies.

5.1 Introduction

Monaco is a neutron/photon, fixed-source Monte Carlo shielding code for the SCALE code package. Monaco uses the SCALE General Geometry Package (SGGP)—the same geometry description as KENO-VI. Monaco has many options available to the user for specifying source distributions, many tally options, and many variance reduction capabilities. Monaco was originally based on the MORSE Monte Carlo code but has been extensively modified to modernize the coding, increase the number of capabilities in terms of sources and tallies, and allow for either multigroup or continuous energy (CE) transport through the use of the new SCALE CE Modular Physics Package (SCEMPP).

Monaco was developed to address a number of long-term goals for the Monte Carlo shielding capabilities in SCALE. The principal goals for this project included (1) unification of geometric descriptions between the SCALE shielding and criticality Monte Carlo codes, (2) implementation of a mesh-based importance map and mesh-based biased source distribution so that automated variance reduction could be used, and (3) establishment of a code using modern programming practices from which to continue future development. The addition of a continuous-energy transport capability is a significant change as well.

Monaco is the key component of the MAVRIC sequence, which also uses Denovo to create the mesh-based importance map and mesh-based biased source distribution for general 3-D automated variance reduction. See the MAVRIC chapter for more information.

5.2 Monaco Capabilities

Monaco has a wide range of source descriptions and tallies for performing general radiation transport calculations. Note that Monaco can work with either the AMPX-based multigroup libraries or the newer AMPX-based CE libraries. Note that for CE calculations, tallies still employ a multigroup energy structure to store and report results.

5.2.1 Source Descriptions

Multiple sources can be defined for a Monaco calculation. Sampling of the different sources can be biased by the user. Each source is specified by its spatial distribution, its energy distribution, its directional distribution, and its strength. Distributions defined by the user can also be biased and can be used multiple times by different sources. The Monaco tallies assume that the sources all have units of particles/second. If the source strengths are given in other units, the user will have to incorporate the proper conversion to the tally results and remember to interpret the results accordingly.

Distributions

Two types of basic distributions are used by Monaco – binned histograms and a set of value/function pairs. The binned histogram type is defined by $n+1$ bin boundaries and *n* values, representing the integrated amount in each bin. For the true distribution$f(x)$, the bin boundaries $[x_0,\ x_1,\ \ldots,\ x_n]$ and the integrated amounts $F_i = \int_{x_{i-1}}^{x_i} f\left(x\right) \mathrm{dx}$ are given. The distribution will be normalized by Monaco after reading. The user can optionally bias a binned histogram distribution by supplying one of the following: the biased sampling distribution amounts, $G_i = \int_{x_{i-1}}^{x_i} g\left(x\right) \mathrm{dx}$; the importance of each bin, I_i; or the suggested weight for each bin, w_i.

Based on what type of input is given, Monaco will compute a properly normalized probability distribution function for sampling. If the importances are given, the sampling distribution is computed as

$$G_i = \frac{I_i F_i}{\sum_i I_i F_i} \tag{5.1}$$

If suggested weights are given, then the sampling distribution is computed as

$$G_i = \frac{\frac{F_i}{w_i}}{\sum_i \frac{F_i}{w_i}} \tag{5.2}$$

for bins with non-zero weight. The sampling distribution for bins with a suggested weight of zero are set to $G_i = 0$. When sampled, particles are assigned a weight of $\frac{F_i}{G_i}$.

The second type of distribution that a user can define is for a series of point values of a function. For a set of $n+1$ point pairs, $(x_i,\ f_i)$ for $i \in [0 \ldots n]$, defining n intervals, a distribution can be made by linearly interpolating between adjacent point pairs. This type of distribution can also be biased by supplying one of the following: the biased sampling distribution function value g_i at each point, the importance of each point, I_i; or the suggested weight for each point, w_i. Similar to above, if importances or weights are given, Monaco computes the biased distribution for sampling. For the value/function point pairs type of distribution, the weight assigned to the sampled particle is a continuous function.

Some commonly used distributions are built into Monaco and can be used by simple keywords. Monaco can produce a graph of any distribution so that the user can verify that the input was entered correctly.

Spatial energy and directional attributes

Each Monaco source is described by three separable components: spatial, energy and directional.

The spatial component of a source in Monaco is simple but very flexible. First, the general shape of the source region is defined in global coordinates. The basic solid shapes and their allowed degenerate cases are listed in Table 5.1. The user can reference any of the defined distributions to describe the source distribution in any coordinate (x, y, and z for cuboids, r and z for cylinders and r for spheres) to use for sampling or leave the source distribution as uniform over each dimension for the solid shape. The source region can be limited by the underlying SGGP geometry variables of unit, media, and mixture. This way, source volumes (or planes, lines, or points) can be defined that are independent or dependent on the model geometry. A cylinder or cylindrical shell region can be oriented with its axis in any direction.

Table 5.1: Available source shapes and their allowed degenerate cases

Shape	Allowable degenerate cases
cuboid	rectangular plane, line, point
cylinder	circular plane, line, point
cylindrical shell	cylinder, planar annulus, circular plane, cylindrical surface, line, ring, point
sphere	point
spherical shell	sphere, spherical surface, point

Monaco samples the source position using either the given distributions or uniformly over the basic solid shape and then uses rejection if any of the optional SGGP geometry limiters have been specified. For sources that are confined to a particular unit, media, or mixture, users should make sure the basic solid shape tightly bounds the desired region for efficient sampling.

For the energy component of each source, either type of distribution described above can be used. Biasing can be used in the energy component of the source as well. The Watt spectrum is a built-in distribution which uses the Froehner and Spencer [FS81] method for sampling. If the defined energy distribution has point(s) that are out of the problem's energy range for a CE problem, these points will be rejected in the source energy sampling and an error message will be generated. The warnings will be suppressed if the number of rejected source points exceeds a pre-defined threshold (1000).

Distributions can be used to define the directional component of the source. A function of the cosine of the polar angle, with respect to some reference direction in global coordinates, can be used by Monaco. If no directional distribution is specified, the default is an isotropic distribution (one directional bin from μ= 1 to μ=1). The default reference direction is the positive z-axis (<0,0,1>).

Monaco mesh source map files

An alternative to specifying the separate spatial and energy distributions, a Monaco mesh source file can be used. A mesh source consists of a 3D Cartesian mesh that overlay the geometry. Each mesh cell has some probability of emitting a source particle, and within each mesh cell, a different energy distribution can be sampled. Position within each mesh cell is sampled uniformly, and the emission direction is sampled from the standard directional distribution. Monaco mesh source files are typically produced by the MAVRIC sequence or by other Monaco calculations (see the mesh source saver option in the source input). For a source constructed from the separable spatial and energy distributions, Monaco can create a mesh source file which can then be visualized using the Mesh File Viewer. This is a convenient way to ensure that the source being used is what was intended.

5.2.2 Tallies

Monaco offers three tally types: point detectors, region tallies, and mesh tallies. Each is useful in determining quantities of interest in the simulation. Any number of each can be used, up to the limit of machine memory. The tallies will compute flux for each group, the total neutron and total photon fluxes, and any number of dose-like responses. A typical dose-like response, *R*, is the integral over energy of the product of a response function, $f(E)$, and the flux, $\phi(E)$.

$$R = \int f(E)\,\phi(E)\,dE \tag{5.3}$$

In multigroup calculations, the total response would be expressed as the sum over all groups $R = \sum f_g \phi_g$. For CE calculations, tallies can be segmented into energy and time bins which can be thought of as "groups". All three of the tally types can be scaled with a constant – for example, to account for units conversions.

Tally statistics

The three Monaco tallies are really just collections of simple and extended tallies for each group, each total, and each group contribution to a response or total response. The simple tally works in the following way: a history score h_i is zeroed out at the start of history i. During the course of the history, when an event occurs during substep j, a score consisting of some contribution c_{ij} weighted by the current particle weight w_{ij} is calculated and added to h_i. At the end of the history, the history score is the total weighted score for each substep j in the history.

$$h_i = \sum_j w_{\mathrm{ij}} c_{\mathrm{ij}} \tag{5.4}$$

Note that the values for the contribution c_{ij} and when it is added to the accumulator are determined by the tally type. At the end of the each history, the history score is added to two accumulators (power sums) - the first accumulator is for finding the tally average, S_1, and the second accumulator is for finding the uncertainty in the tally average, S_2.

$$S_1 = \sum_i h_i \tag{5.5}$$

$$S_2 = \sum_i h_i^2 \tag{5.6}$$

At the end of all N histories, the second sample central moment is found from the power sums

$$m_2 = \frac{S_2}{N} - \frac{S_1^2}{N^2} \tag{5.7}$$

and then the tally average is computed as $\overline{x} = \frac{S_1}{N}$ and the uncertainty in the tally average is $u = \sqrt{\frac{m_2}{N}}$.

The extended tally uses four accumulators – the first and second are the same as the simple tally – with the third and fourth accumulators used for finding the variance of the variance (VOV). These extra accumulators, S_3 and S_4, are calculated as

$$S_3 = \sum_i h_i^3 \tag{5.8}$$

$$S_4 = \sum_i h_i^4 \tag{5.9}$$

At the end of all N histories, the tally average $\overline{x}$ and uncertainty in the tally average u are found in the same way as a simple tally. For the VOV calculation, the third and fourth sample central moments are found as

At the end of all N histories, the tally average $\overline{x}$ and uncertainty in the tally average u are found in the same way as a simple tally. For the VOV calculation, the third and fourth sample central moments are found as

$$m_3 = \frac{S_3}{N} - \frac{3S_1S_2}{N^2} + \frac{2S_1^3}{N^3} \tag{5.10}$$

$$m_4 = \frac{S_4}{N} - \frac{4S_1S_3}{N^2} + \frac{6S_1^2S_2}{N^3} - \frac{3S_1^4}{N^4} \tag{5.11}$$

and then the VOV [PFB97] and figure-of-merit (FOM) are found using

$$\text{VOV} = \frac{m_4 - m_2^2}{Nm_2^2} \tag{5.12}$$

$$\text{FOM} = \frac{1}{\left(\frac{u}{\overline{x}}\right)^2 T} \tag{5.13}$$

where T is the calculation time (in minutes).

Extended tallies are used for the total neutron flux, total photon flux and any responses for the Monaco tallies. Simple tallies are used for each group's flux and each group's contribution to a response.

Detailed, group-wise results for each tally are saved to separate files at the end of each batch of particles. Users can view these files (in the SCALE temporary directory) as the Monaco simulation progresses. Summaries of the extended tallies appear in the final Monaco output file.

Statistical tests

Statistical tests are performed on the extended tallies at the end of each batch. Results for each batch are stored in files and the results for the final batch are shown in the main output tally summary. The six tests are:

	Quantity	Test	Goal	Within
1.	mean	relative slope of linear fit	= 0.00	± 0.10
2.	standard deviation	exponent of power fit	= -0.50	$R^2 > 0.99$
3.	relative uncertainty	final value	< 0.05	
4.	relative VOV	exponent of power fit	= -1.00	$R^2 > 0.95$
5.	relative VOV	final value	< 0.10	
6.	figure-of-m erit	relative slope of linear fit	= 0.00	± 0.10

For the tests that are fit to a function with respect to batch (1, 2, 4, and 6), only the last half of the simulation is used. The basis for these tests is that in a well-behaved Monte Carlo, the mean should not increase or decrease as a function of the number of histories (N), the standard deviation should decrease with $\frac{1}{\sqrt{N}}$, the variance of the variance should decrease with $\frac{1}{N}$ and the figure-of-merit should neither

increase or decrease as a function of the number of histories (proportional to time). For tests 2 and 4, the coefficient of determination, R^2, from a forced fit to a function with the right exponent is used as the tally test.

Point detector tallies

Point detectors are a form of variance reduction in computing the flux or response at a specific point. At the source emission site and at every interaction in the particle's history, an estimate is made of the probability of the particle striking the position of the point detector. For each point detector, Monaco tallies the uncollided and total flux for each energy group, the total for all neutron groups, and the total for all photon groups. Any number of optional dose-like responses can be calculated as well.

Multigroup

After a source particle of group g is started, the distance R between the source position and the detector position is calculated. Along the line connecting the source and detector positions, the sum of the distance sj through each region j multiplied by the total cross section $\Sigma_j^g$for that region is also calculated. The contribution cg to the uncollided flux estimator is then made to the tally for group g.

$$c_g = \frac{1}{4\pi R^2} \exp\left(-\sum_j s_j \Sigma_j^g\right) \tag{5.14}$$

Continuous Energy

After a source particle with energy *E* is started, the distance *R* between the source position and the detector position is calculated. For each bin g of the tally energy structure, a specific energy E_g is sampled uniformly within the bin. Along the line connecting the source and detector positions, the sum of the distance *sj* through each region *j* multiplied by the total cross section $\Sigma_j\left(E_g\right)$ for that region. The contribution *cg* to the uncollided flux estimator is then made to the tally for group g. total cross section $\Sigma_j\left(E\right)$:

$$c_g = \frac{1}{4\pi R^2}\exp\left(-\sum_j s_j \Sigma_j\left(E\right)\right) \tag{5.15}$$

Only source particles contribute to the uncollided flux tally. At each interaction point during the life of the particle, similar contributions are made to each of the tallies. For each group *g* that the particle could scatter into and reach the detector location, a contribution is made that also includes the probability to scatter from the current direction towards the detector and having the energy change from group *g* to group g.

This type of tally is costly, since ray-tracing through the geometry from the current particle position to the detector location is required many times over the particle history. Point detectors should be located in regions made of void material, so that contributions from interactions arbitrarily close to the point detector cannot overwhelm the total estimated flux (as $\frac{1}{4\pi R^2 \to \infty}$).

Care must be taken in using point detectors in deep penetration problems to ensure that the entire phase space that could contribute has been well sampled—so that the point detector is not underestimating the flux by leaving out areas far from the source but close to the point detector position. One way to check this is by examining how the tally average and uncertainty change with each batch of particles used in the simulation. Large fluctuations in either quantity could indicate that the phase space is not being sampled well.

Region tallies

Region tallies are used for calculating the flux and/or responses over one of the regions listed in the SGGP geometry. Both the track-length estimate of the flux and the collision density estimate of the flux are calculated—and for each, the region tally contains simple tallies for finding flux in each group, the total neutron flux, and the total photon flux. For each of the optional response functions, the region tally also contains simple tallies for each group and the total response.

For the track-length estimate of flux, each time a particle of energy E moves through the region of interest, a contribution of l (the length of the step in the region) is made to the history score for the simple tally for flux for tally group g. The same contribution is made for the history score for the simple tally for total particle flux, neutron or photon, depending on the particle type.

If any optional response functions were requested with the tally, then the contribution of $\mathrm{lf}\left(E\right)$is made for the response group, where $f\left(E\right)$ is the response function value for energy E. The history score for the total response function is also incremented using $\mathrm{lf}\left(E\right)$.

At the end of all of the histories, the averages and uncertainties of all of the simple tallies for fluxes are found for every group and each total. These results then represent the average track-length over the region. To determine flux, these results are divided by the volume of the region. If the volume V of the region was not given in the geometry input nor calculated by Monaco, then the tally results will be just the average track lengths and their uncertainties. A reminder message is written to the tally detail file if the volume of the region was not set.

For the collision density estimate of the flux, each time a particle of energy E has a collision in the region of interest, a contribution of $\frac{1}{\Sigma}$ (the reciprocal of the total macroscopic cross section) is made to the history scores for the simple tally for flux for tally energy group *g* and for the total particle flux. At the end of the simulation, the averages and uncertainties of all of the simple tallies for every group flux and total flux are found and then divided by the region volume, if available.

Similar to the point detector tallies, region tallies produce a file listing the tally average and uncertainty at the end of each batch of source particles (a *.chart file). This file can be plotted using the simple 2-D plotter (ChartPlot) to observe the tally convergence behavior.

Mesh tallies

For a D Cartesian mesh or a cylindrical mesh (independent of the SGGP geometry), Monaco can calculate the track-length estimate of the flux. Since the number of cells (voxels) in a mesh can become quite large, the mesh tallies are not updated at the end of each history but are instead updated at the end of each batch of particles. This prevents the mesh tally accumulation from taking too much time but means that the estimate of the statistical uncertainty is slightly low.

Like the other tallies, mesh tallies can calculate optional response functions.

Since a mesh tally consists of many actual tallies, the statistical tests are a bit more complex than for the region and point detector tallies. Several statistical quantities and tests are used in Monaco similar to those in several recent studies [KS11][KI11] which look at a distribution of relative variances over the mesh tally. In Monaco, the basis of the statistical tests center on the distribution of relative uncertainties and its mean, $\overline{r}$, of the voxels (V) with score.

$$\overline{r} = \frac{1}{V} \sum R_i \tag{5.16}$$

where R_i is the relative uncertainty of the flux or dose in voxel i. If every voxel has been sampled well and its relative uncertainty $R_i \propto \frac{1}{\sqrt{N}}$, then the mean relative uncertainty of the voxels should also behave as $\frac{1}{\sqrt{N}}$. The variance of the mean relative uncertainty can be calculated and a figure of merit (FOM) for the mesh tally can be constructed using

$$FOM = \frac{1}{\overline{r}^2 T} \tag{5.17}$$

with the time T in minutes. The four tests measure over the simulation: 1) if ζ, the fraction of voxels with non-zero score, is constant; 2) if the mean relative uncertainty is decreasing as $\frac{1}{\sqrt{N}}$ (as measured by the coefficient of determination, R^2, of a fit to a curve with power of -0.5); 3) if the variance of the mean relative uncertainty is decreasing with $\frac{1}{N}$; and 4) if the FOM is constant.

	Quantity	Test	Goal	Within
1.	ζ, fraction with score	relative slope of linear fit	= 0.00	± 0.10
2.	$\overline{r}$, mean relative uncertainty	exponent of power fit	= -0.50	$R^2 > 0.99$
3.	variance of $\overline{r}$	exponent of power fit	= -1.00	$R^2 > 0.95$
4.	figure-of-merit	exponent of power fit	= 0.00	± 0.10

For non-uniform meshes (especially cylindrical), these tests may not be the best measure of performance since different size voxels will have a wider variety of relative uncertainties. The user is also cautioned that if there are individual voxels within the mesh tally that have relative uncertainties that are not decreasing as $\frac{1}{\sqrt{N}}$, then the mesh tally statistical tests will not be meaningful. It is ultimately up to the user to decide if the mesh tally is performing well (is the goal

of the mesh tally just to calculate dose, not flux?; are all spatial areas of the mesh tally equally important?; are all magnitudes of the flux or response values equally important?; etc.)

Mesh tallies can be viewed with the Mesh File Viewer, a Java utility that can be run from GeeWiz (on PC systems) or can be run separately (on any system). The Mesh File Viewer will show the flux for each group, the total flux for each type of particle and the optional responses. Uncertainties and relative uncertainties can also be shown for mesh tallies using the Mesh File Viewer. For more information on the Mesh File Viewer, see its on-line documentation.

5.2.3 Continuous Energy Transport

Using multigroup data in Monte Carlo transport calculations is generally sufficient for most problems (both shielding and criticality). Many of the reaction cross sections vary slowly with energy, so energy "groups" can be made with one set of properties for the group. Multigroup treatments can further simplify radiation transport by combining the different types of reactions that can occur into a simple scattering matrix – particles then have certain probabilities to scatter from their current energy group to another energy group. If the user is not interested in knowing which specific type of interaction happened at each collision, this simplification can increase calculation efficiency.

One major drawback of the multigroup approach is in representing discrete gammas, such as the decay radiation from common isotopic sources. Consider a simple shielding simulation using cobalt-60. This isotope gives off two high-energy gamma rays when it decays (1173230 eV with intensity 99.85% and 1332490 eV with intensity 99.9826%). In the SCALE multigroup calculations, a cobalt-60 source spectrum is represented by a broad pdf, controlled by the group structure. This is shown in Fig. 5.1. for the fine 47-group structure and the broad 19-group structure.

Fig. 5.1: The multigroup representation of a cobalt-60 source.

Note that in both group structures, 1.33 MeV is a group boundary, so the 1332490 eV line is represented by group that covers higher energies. The cross section for that group is lower than the cross section for the specific line, so multigroup transport calculations will tend to overestimate the number of photons penetrating a shield, which will overestimate dose rates.

Using CE and the two multigroup libraries, the total cross sections for the cobalt lines are listed in Table 5.2. Fig. 5.2. shows the total cross section of photons in tungsten, in both CE and the two SCALE multigroup structures. On the whole, the multigroup data represents the CE data well. Fig. 5.3. shows the same cross section information near the two cobalt lines, which shows how the multigroup cross sections average over quite large energy ranges.

Table 5.2: Total macroscopic cross section in tungsten (/cm).

	1173230 eV	1332490 eV
SCALE CE	1.03353	0.94864
SCALE 47	1.09066	0.92743
SCALE 19	1.05167	0.89289

The small differences in cross section can make large differences in the transport. Consider just 5 cm of tungsten. Using the cross sections in Table 5.2, the attenuation ($e^{-\mu x}$) of either line can vary by 30%.

In addition to source representation problems, multigroup transport is not adequate for applications where line spectra are measured. Because of the group structure, tally results will be averaged out within a group. With the fixed boundaries, specific lines in the tallies will not be able to be seen. For examples, in the 19-group library, there is no group around the 511 keV annihilation gammas – they are averaged in with other photons from 400 to 600 keV. No multigroup structure could contain thin groups around every line of interest.

Fig. 5.2: Photon total cross section in tungsten. The energies of the cobalt-60 are displayed as lines at 1173230 and 1332490 eV.

A sample problem involving a cobalt source and a slab of tungsten will compare the use of continuous-energy transport to multigroup transport, to demonstrate the large difference in results for single-line sources. For distributions, differences between multigroup and continuous-energy may not be very significant.

5.3 Monaco Input Files

The input file for Monaco consists of two lines of text ("=monaco" command line and one for the problem title) and then several blocks, with each block starting with "read xxxx" and ending with "end xxxx". There are three blocks that are required and seven blocks that are optional. The cross section and geometry blocks must be listed first and in the specified order. Other blocks may be listed in any order.

Blocks (must be in this order):

- Cross Sections – (required) lists the cross-section file and the mixing table information
- Geometry – (required) SCALE general geometry description

Fig. 5.3: Photon total cross section in tungsten, near the cobalt lines. The energies of the cobalt-60 are displayed as lines at 1173230 and 1332490 eV.

- Array – optional addition to the above geometry description
- Volume – optional calculation or listing of region volumes
- Plot – create 2D slices of the SGGP geometry

Other Blocks (any order, following the blocks listed above):

- Definitions – defines locations, response functions, grid geometries, cylindrical mesh geometries, energy bin boundaries, time bin boundaries and various distributions used by other blocks
- Source – (required) description of multiple sources; with the spatial, energy, and directional distributions and particle type for each
- Tallies – description of what to calculate: point detector tallies, region tallies, or mesh tallies
- Parameters – how to perform the simulation (random number seed, how many histories, etc.)
- Biasing – data for reducing the variance of the simulation

The physical model blocks (Geometry, Array, Volume and Plot) follow the standard SCALE format. See the other SCALE references as noted in the following sections for details.

For the other six blocks, scalar variables are set by "keyword=value", fixed length arrays are set with "keyword $value_1$ … $value_N$", variable length arrays are set with "keyword $value_1$ … $value_N$ end", and some text and filenames are read in as quoted strings. Single keywords to set options are also used in some instances. The indention, comment lines, and upper/lower case shown in this document are not required—they are used in the examples only for clarity. Except for strings in quotes (like filenames), SCALE is not case sensitive.

After all of the blocks are listed, a single line with "end data" should be listed. A final "end" should also be listed, to signify the end of all Monaco input. See Table 5.3 for an overview of the Monaco input file structure.

5.3.1 Cross sections block

Monaco does its own mixing, so it needs a mixing table. For each element of each mixture, an identifier and a number density must be supplied. These can be found in the output of whatever sequence was used to make the cross-section file, such as CSAS-MG. Two coupled neutron/photon multigroup libraries were created specifically for shielding problems from ENDF/B-VII.0 data—the v7-200n47g fine-group and the v7-27n19g coarse-group libraries. CE libraries made from ENDF/BVII.0 are also available in SCALE.

Table 5.3: Overall input format for Monaco

Input File	Comment
=monaco	
S	name
o	a
m	m
e	e
t	o
i	f
t	s
l	e
e	q
f	u
o	e
r	n
t	c
h	e
i	
s	t
p	i
r	t
o	l
b	e
l	
e	L
m	i
read	s
crossSections	t
	o
.	f
.	i
.	s
end	o
crossSections	t
read	o
geometry	p
	e
.	s
.	/
.	m
end	i
geometry	x
read	t
array	u
	r
.	e
.	s
.	
end	[
array	r
read	e
volume	q
	u
.	i
.	r
.	e
end	d
volume	b
read	l
plot	o
	c
.	k
	]

For example, if CSAS-MG was used to produce an AMPX file using the following input,

```
=csas-mg

D
e
m
o
n
s
t
r
a
t
i
o
n
p
r
o
b
l
e
m
,
t
h
r
e
e
m
i
x
t
u
r
e
s

v7
-200
n47
g
read
 composition

u
o2   1 0
.2 293
.0 92234 0
.0055 92235 3
.5 92238 96
.4945 end

s
s304 2 1
.0 293
.0 end
```

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(continued from previous page)

```
h2
o   4 1
.0 293
.0 end
end
 composition
end
```

in addition to creating an AMPX file, the output would include a tables similar to

```
m
i
x
i
n
g
t
a
b
l
e
(
T
H
R
E
A
D
= 00
)

e
n
t
r
y
m
i
x
t
u
r
e
i
s
o
t
o
p
e
n
u
m
b
e
r
d
e
n
s
i
t
```

(continues on next page)

(continued from previous page)

```
    1        1         92234     2
.73451
E
-07              92234              293
.0
    2        1         92235     1
.73272
E
-04              92235              293
.0
    3        1         92238     4
.71674
E
-03              92238              293
.0
    4        1          8016     9
.78057
E
-03               8016              293
.0


m
i
x
i
n
g
t
a
b
l
e
(
T
H
R
E
A
D
= 00
)

e
n
t
r
y
m
i
x
t
u
r
e
i
s
o
t
o
p
e
n
u
```

(continues on next page)

(continued from previous page)

```
    1       2         6000     3
.18488
E
-04              6000             293
.0
    2       2        14028     1
.57010
E
-03             14028             293
.0
    3       2        14029     7
.97625
E
-05             14029             293
.0
    4       2        14030     5
.26416
E
-05             14030             293
.0
    5       2        15031     6
.94688
E
-05             15031             293
.0
    6       2        24050     7
.59178
E
-04             24050             293
.0
    7       2        24052     1
.46400
E
-02             24052             293
.0
    8       2        24053     1
.66006
E
-03             24053             293
.0
    9       2        24054     4
.13224
E
-04             24054             293
.0
   10       2        25055     1
.74072
E
-03             25055             293
.0
   11       2        26054     3
.42190
E
-03             26054             293
.0
   12       2        26056     5
.37166
E
-02             26056             293
.0
```

(continues on next page)

(continued from previous page)

```
   13       2        26057     1
.24055
E
-03             26057             293
.0
   14       2        26058     1
.65094
E
-04             26058             293
.0
   15       2        28058     5
.26873
E
-03             28058             293
.0
   16       2        28060     2
.02951
E
-03             28060             293
.0
   17       2        28061     8
.82212
E
-05             28061             293
.0
   18       2        28062     2
.81288
E
-04             28062             293
.0
   19       2        28064     7
.16357
E
-05             28064             293
.0


m
i
x
i
n
g
t
a
b
l
e
(
T
H
R
E
A
D
= 00
)
```

(continues on next page)

(continued from previous page)

```
e
n
t
r
y
m
i
x
t
u
r
e
i
s
o
t
o
p
e
n
u
m
b
e
r
d
e
n
s
i
t
y
n
e
w
i
d
e
n
t
i
f
i
e
r
e
x
p
l
i
c
i
t
t
e
m
p
e
r
a
t
u
r
```

(continues on next page)

(continued from previous page)

```
    1       4         1001     6
.67531
E
-02              1001             293
.0
    2       4         8016     3
.33765
E
-02              8016             293
.0
```

which can be used to construct the Monaco cross-section block mixing table.

```
read
 crossSections

a
m
p
x
F
i
l
e
U
n
i
t
=4

m
i
x
t
u
r
e 1

e
l
e
m
e
n
t    92234 2.73451E-07

e
l
e
m
e
n
t    92235 1.73272E-04

e
l
e
m
e
n
t    92238 4.71674E-03
```

(continues on next page)

(continued from previous page)

```
e
l
e
m
e
n
t     8016 9.78057E-03
    end
 mixture

m
i
x
t
u
r
e 2

e
l
e
m
e
n
t     6000 3.18488E-04

e
l
e
m
e
n
t    14028 1.57010E-03

e
l
e
m
e
n
t    14029 7.97625E-05

e
l
e
m
e
n
t    14030 5.26416E-05

e
l
e
m
e
n
t    15031 6.94688E-05
```

(continues on next page)

(continued from previous page)

```
e
l
e
m
e
n
t    24050 7.59178E-04

e
l
e
m
e
n
t    24052 1.46400E-02

e
l
e
m
e
n
t    24053 1.66006E-03

e
l
e
m
e
n
t    24054 4.13224E-04

e
l
e
m
e
n
t    25055 1.74072E-03

e
l
e
m
e
n
t    26054 3.42190E-03

e
l
e
m
e
n
t    26056 5.37166E-02
```

(continues on next page)

```
e
l
e
m
e
n
t    26057 1.24055E-03
```

(continued from previous page)

```
e
l
e
m
e
n
t    26058 1.65094E-04

e
l
e
m
e
n
t    28058 5.26873E-03

e
l
e
m
e
n
t    28060 2.02951E-03

e
l
e
m
e
n
t    28061 8.82212E-05

e
l
e
m
e
n
t    28062 2.81288E-04

e
l
e
m
e
n
t    28064 7.16357E-05
    end
 mixture

m
i
x
t
u
r
e 4
```

(continues on next page)

(continued from previous page)

```
e
l
e
m
e
n
t     1001 6.67531E-02

e
l
e
m
e
n
t     8016 3.33765E-02
    end
 mixture
end
 crossSections
```

For a CE calculation, instead of the keyword "ampxFileUnit=" (which refers to a given AMPX library), the keyword "ceLibrary=" should be used with a CE library name, enclosed in quotes. Also for CE, a default temperature can be set before any mixtures are defined using the "ceTempDefault=" temperature (in Kelvins). With each mixture, a specific temperature can be set using "temperature."

Other keywords that can be used in the cross-section block for multigroup problems include flags to turn on printing of different aspects of the cross-section mixing process ("printTotals", "printScatters", "printAngleProb", "printFissionChi", "printExtra", and "printLegendre"). The keyword "fullyCoupled" can be used to specify all groups to be treated as primary groups. These keywords do not work in CE problems since the point wise data contain an enormous number of points.

Users are encouraged to use Monaco by running the MAVRIC sequence, which creates the cross-section mixing table automatically, for both multigroup and CE calculations.

5.3.2 Geometry block

The geometry input uses the standard SGGP, similar to KENO-VI. Input instructions can be found in *Geometry Data* in the KENO-VI chapter of the SCALE manual.

Shielding calculations (Monaco, MAVRIC, SAS4) differ from their criticality cousins (KENO V.a, KENO-VI) in a very special way—sources and detectors can be located outside of the materials where the transport takes place. To accommodate this fact in Monaco and MAVRIC, make sure that a void region (a media record using mixture 0) surrounds the source area and any point detectors, if they are not located in a region of the actual geometry.

For example, if the objective is to calculate the effectiveness of a simple slab shield, the model geometry would consist of just one slab of material. The source would be on one side of the slab, and a detector would be on the other side of the slab. In Monaco (and the MAVRIC sequence), the input should list at least two regions: (1) the slab itself and (2) a void region outside of the slab containing both the source and detector positions.

Monaco tracks particles through the SGGP geometry as well as other geometries used for mesh tallies or mesh importance maps. Because Monaco must track through all of these geometries at the same time, users should not use the reflective boundary capability in the SGGP geometry.

The graphical user interfaces GeeWiz and Keno3D can be used on Windows platforms to develop and view the geometry.

5.3.3 Array, volume, and plot blocks

Geometry array input uses the standard SGGP, similar to KENO-VI. Input instructions can be found in KENO-VI chapter on *Array Data* of the SCALE manual.

Volumes of various geometry regions are used to calculate fluxes for those regions. Volumes can be input as part of the geometry input block above, or calculated by the SGGP using one of two different methods. See KENO-VI chapter on *Volume Data* for instructions.

The "read plot" block allows users to create a 2-D character or color plots of slices through a specified portion of the 3-D geometrical representation of the problem. These images can be saved as *.png files. For more information, see the KENO-VI chapter on *Plot Data*.

5.3.4 Definitions block

The definitions block defines different types of data (locations, detector response functions, grid geometries, cylindrical geometries, distributions, energy bin boundaries and time bin boundaries) that are used by some of the other blocks in Monaco. Individual data can be listed in any order. Identification numbers must be positive integers and unique within that type of data. Each type of data begins with a keyword and ends with an "end" and that same keyword. All of the different data types can have an optional title using the keyword "title=".

```
read
 definitions

l
o
c
a
t
i
o
n 43

...
    end
 location

r
e
s
p
o
n
s
e 45

...
    end
 response

d
i
s
t
r
i
b
```

(continues on next page)

```
u
t
i
o
n 1
```

(continued from previous page)

```
...
    end
 distribution

r
e
s
p
o
n
s
e 12

...
    end
 response
end
 definitions
```

Locations

Locations ("location") require an identification number and the physical position in global coordinates using the "position" keyword (a fixed length array). A position is specified by listing its x, y, and z coordinates.

```
l
o
c
a
t
i
o
n  1

t
i
t
l
e
="Radial detector - close to surface"

p
o
s
i
t
i
o
n 162
.0 0
.0 0
.0
end
 location
```

(continues on next page)

(continued from previous page)

```
l
o
c
a
t
i
o
n  2
p
o
s
i
t
i
o
n 0
.0 0
.0 295
.6   end
 location

l
o
c
a
t
i
o
n  3

t
i
t
l
e
=
"
C
o
r
n
e
r
d
e
t
e
c
t
o
r
"

p
o
s
i
t
i
o
n 162
.0 0
.0 295
```

(continues on next page)

(continued from previous page)

```
end
 location

l
o
c
a
t
i
o
n 105
p
o
s
i
t
i
o
n   0
.0 0
.0 385
.6   end
 location

l
o
c
a
t
i
o
n 106
p
o
s
i
t
i
o
n 252
.0 0
.0 385
.6   end
 location
```

Response functions

Response functions ("response") require an identification number and information on how to build an energy dependent response function. There are three basic types of responses: 1) the general user-defined response, 2) a response based on cross-section data, and 3) a response based on a specific flux-to-dose conversion factor. For multigroup calculations, a fourth type of a response simply listing multigroup values is also available. Responses must be defined as either a neutron response or a photon response.

Type 1. A general user-defined response function can be either a binned histogram function (n+1 energies and n values) or a set of value/function pairs that will be linearly interpolated (n+1 energies and n+1 values). The energies (in eV) are set using the "bounds … end" keyword. The response values

are entered with the "values … end" keyword. The energies can be entered from low energy to high energy order or the traditional high energy to low energy order but must be monotonic. The values array of the response is interpreted to correspond to the order of the bounds array. These two examples

```
r
e
s
p
o
n
s
e 11

t
i
t
l
e
="user-defined response, histogram"

n
e
u
t
r
o
n

b
o
u
n
d
s 1
e7   8
e6   6
e6   4
e6   2
e6   1
e5 end

v
a
l
u
e
s    1
.0   0
.8   0
.6   0
.4   0
.2    end
end
 response

r
e
s
p
o
n
s
e 12
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="user-defined response, value/function pairs"

p
h
o
t
o
n

b
o
u
n
d
s  1
e5 2
e6 4
e6 6
e6 8
e6 1
e7 end

v
a
l
u
e
s 0
.01 0
.2 0
.4 0
.6 0
.8 1
.0 end
end
 response
```

are shown in Fig. 5.4 and Fig. 5.5.

Type 2. Data from the cross-section library can also be used to define a response, for example in finding reaction rates. For the cross section (with units of barns) for a single isotope, the user specifies a material/ZAID/MT combination. The keyword "macro" can be used to multiply the cross section by the atom density of the ZAID in the material (which converts the units of the response from barns to /cm). Users can also specify just the material and MT numbers, to produce the macroscopic cross section of reaction MT for the entire material (with units of /cm). A partial list of common MT numbers is shown in Table F23.3.2 (the full list is in XSECLIB M04, Appendix B). To match some other sequences in SCALE, users can also use text strings to specify the ZAID and MT by using keywords "nuclide=" (for example, nuclide=U-235) and "reaction=" (for example reaction=fission). If the user requested a microscopic cross section response for a reaction in a CE problem, the response will be generated for the nuclide from the AMPX CE libraries even if the nuclide itself is not included in any of the material definitions in the problem. Available reaction lists depend on the

Fig. 5.4: Histogram-type response.

Fig. 5.5: Value/function pair response.

nuclide and the list will be printed as a warning message in the output if a non-existing reaction is requested.

```
read
 composition

u
o2 7 1
.0 293
.0 end
end
 composition

...
read
 definitions

r
e
s
p
o
n
s
e 41

t
i
t
l
e
=
"
g
e
t
t
h
e
m
i
c
r
o
s
c
o
p
i
c
(
b
)
f
o
r 235
"

n
e
u
t
r
o
n
```

(continues on next page)

(continued from previous page)

```
m
a
t
e
r
i
a
l
=7
Z
A
I
D
=92235
M
T
=18
    end
 response

r
e
s
p
o
n
s
e 43

t
i
t
l
e
=
"
g
e
t
t
h
e
m
a
c
r
o
s
c
o
p
i
c
(
/
c
m
)
f
o
r 235
"
```

(continues on next page)

(continued from previous page)

```
n
e
u
t
r
o
n

m
a
t
e
r
i
a
l
=7
Z
A
I
D
=92235
M
T
=18

m
a
c
r
o
    end
 response

r
e
s
p
o
n
s
e 45

t
i
t
l
e
=
"
g
e
t
t
h
e
m
a
c
r
o
s
c
```

(continues on next page)

(continued from previous page)

```
n
e
u
t
r
o
n

m
a
t
e
r
i
a
l
=7
M
T
=18
    end
 response
end
 definitions
```

For the examples above, response 41 is shown in Fig. 5.6. and Fig. 5.7. for both MULTIGROUP and CE.

Table 5.4: Common MT (reaction) numbers for responses

MT	Description	MT	Description
1	Total cross section	501	Total photon interaction cross section
18	Total fission cross section	502	Photon coherent scattering
27	Absorption cross section (MT=18 and 101)	504	Photon incoherent scattering
101	Neutron disappearance	516	Pair production, nuclear and electron field
102	(n,γ) radiative capture cross section	518	Photofission (γ,f)
103	(n,p) cross section	522	Photoelectric
104	(n,^{2}H) cross section		
105	(n,^{3}H) cross section		
106	(n,^{3}He) cross section		
107	(n,^{4}He) cross section		
1452	Product of ν times the fission cross section		

Type 3. Flux-to-dose conversion factors are a little different in multigroup and continuous-energy implementations. The AMPX multigroup shielding libraries contain neutron and photon dose responses from several sources. These have been processed by the AMPX system (the jergens module). To form the multigroup values for the libraries, the original data was extrapolated to cover the entire energy range of the shielding libraries and was then collapsed into the group structures using a weighting spectrum. These dose responses can be accessed through Monaco/MAVRIC by defining a response object that uses the keyword "specialDose=" and then providing the MT number of the particular response. The dose responses available in the shielding libraries in are shown in Table 5.5. Note that the coupled responses in SCALE 6.1 are no longer used by Monaco, since responses are now defined to be either a neutron response or a photon response. When using the "specialDose=" keyword, the

Fig. 5.6: Multigroup ^{235}U total fission cross section.

Fig. 5.7: CE ^{235}U total fission cross section.

"neutron" or "photon" designation is ignored, since the particle type is inherent with the MT number.

```
read
 definitions

r
e
s
p
o
n
s
e 1

s
p
e
c
i
a
l
D
o
s
e
=9031
    end
 response
end
 definitions
```

Table 5.5: Flux-to-Dose conversion factor MT numbers

	Neutron		Photon	
Response	MT	Units	MT	Units
Henderson conversion factors	9027	(rad/h)/(n/cm^2/s)	9502	(rad/h)/(p/cm^2/s)
Claiborne-Trubey conversion factors			9503	(rad/h)/(p/cm^2/s)
ANSI standard (1977) flux-to-dose-rate factors	9029	(rem/h)/(n/cm^2/s)	9504	(rem/h)/(p/cm^2/s)
ANSI standard (1991) flux-to-dose-rate factors	9031	(rem/h)/(n/cm^2/s)	9505	(rem/h)/(p/cm^2/s)
ICRU-44 Table B.3 (air) Kerma	9032	(Gy/h)/(n/cm^2/s)		
	9033	(rad/h)/(n/cm^2/s)		
ICRU-57 Table A.21 (air) Kerma			9506	(Gy/h)/(p/cm^2/s)
			9507	(rad/h)/(p/cm^2/s)
Ambient dose equivalent (ICRU-57)	9034	(Sv/h)/(n/cm^2/s)	9508	(Sv/h)/(p/cm^2/s)
	9035	(rem/h)/(n/cm^2/s)	9509	(rem/h)/(p/cm^2/s)
Effective dose (ICRU-57)	9036	(Sv/h)/(n/cm^2/s)	9510	(Sv/h)/(p/cm^2/s)
	9037	(rem/h)/(n/cm^2/s)	9511	(rem/h)/(p/cm^2/s)

The standard flux-to-dose conversion factors have not been made part of the continuous-energy libraries. Rou-

tines have been added to the Monaco code base to generate data points to allow users to define responses based on the original references. Note that the responses in these references were defined over different energy ranges, as shown in Table 5.6.

Table 5.6: Energy ranges of the original Flux-to-Dose responses

Response	Neutron Energy Range (MeV)		Photon Energy Range (MeV)	
Henderson conversion factors	0.01	18	0.01	10
Claiborne-Trubey conversion factors			0.02	16
ANSI standard (1977) flux-to-dose-rate factors	2.5E-08	20	0.01	15
ANSI standard (1991) flux-to-dose-rate factors	2.5E-08	14	0.01	12
ICRU-44 Table B.3 (air) Kerma	2.5E-08	29		
ICRU-57 Table A.21 (air) Kerma			0.01	10
Ambient dose equivalent (ICRU-57)	1.0E-09	20.1	0.01	10
Effective dose (ICRU-57)	1.0E-09	18	0.01	10

The keyword "doseData=" can be used to create a response using the original, point-wise data (except for Claiborne-Trubey where the original data is a histogram). Data points are also extrapolated to cover the energy range of 10^{-5} to 2×10^{7} eV for neutrons and up to 20 MeV for photons. (The optional keyword "noExtrapolation" can be used to get just the original data without the extrapolations.) The final response is formed by interpolating (lin-lin) between these points. For multigroup problems, these keywords will collapse the original data (with or without extrapolation) into a multigroup structure but without the weighting function used to create the dose factors in the multigroup libraries. This will not match the multigroup responses in the those libraries.

```
read
 definitions

r
e
s
p
o
n
s
e 1

d
o
s
e
D
a
t
a
=9031
    end
 response

r
e
s
p
o
n
s
e 1
```

(continues on next page)

(continued from previous page)

```
d
o
s
e
D
a
t
a
=9031
n
o
E
x
t
r
a
p
o
l
a
t
i
o
n
    end
 response
end
 definitions
```

As an example of the various forms of a flux-to-dose conversion factor, the ANSI 1991 values (MT=9031 and 9505) are shown in Fig. 5.8 through Fig. 5.11.

Fig. 5.8: ANSI 1991 neutron CE (left is log-log, right is linear-linear)

The use of the "specialDose=" and "doseData=" keywords is summarized in Table 5.7. Users should understand that the only way to get the 'true' response described in the original references is to use the "doseData=" and "noExtrapolation" keywords. The traditional approach in SCALE has been to extrapolate the original data over the entire energy range of the problem, yielding higher dose rates than the 'true' response would.

Fig. 5.9: ANSI 1991 neutron MULTIGROUP (left is log-log, right is linear-linear)

Fig. 5.10: ANSI 1991 photon CE (left is log-log, right is linear-linear)

Fig. 5.11: ANSI 1991 photon MULTIGROUP (left is log-log, right is linear-linear)

Table 5.7: Use of the "specialDose=" and "doseData=" keywords.

keyword(s)	Multi-Group (MG)	Continuous Energy (CE)
specialDose=*MT*	uses pre-computed responses contained in the MG library: data points from reference, extrapolated to energy range of the library and collapsed to the library group structure using a weighting spectrum	this keyword is not allowed since there are no pre-computed dose responses contained within the CE libraries
doseData=*MT*	data points from reference, extrapolated over the range of 1.0d-11 to 20.0 MeV and collapsed to the library group structure without a weighting spectrum	data points from reference, extrapolated over the range of 1.0d-11 to 20.0 MeV
doseData=*MT* noExtrapolation	data points from reference and collapsed to the library group structure without a weighting spectrum	data points from reference using only the original energy range

Type 4. For multigroup calculations, since the energy structure is already known, a response can be defined by listing just the values for each group using the keyword "values ... end". The array length of this type of response should match the number of energy groups for that particle type in the cross-section library. Values should be entered in the standard multigroup order – from high energy to low energy. The shortcut keyword "unity" places a value of 1.0 as the response for each group.

```
r
e
s
p
o
n
s
e 19

t
i
t
l
e
="Total Photon Dose at Each Detector Point Location (ANSI 9504)"

p
h
o
t
o
n

v
a
l
u
e
s                          1
 16200
E
-05  8
.74457
E
```

(continues on next page)

(continued from previous page)

```
         6
.35058
E
-06  5
.39949
E
-06  4
.60165
E
-06  3
.95227
E
-06  3.45885E-06
         3
.01309
E
-06  2
.62001
E
-06  2
.19445
E
-06  1
.82696
E
-06  1.51490E-06
         1
.15954
E
-06  8
.70450
E
-07  6
.21874
E
-07  3
.70808
E
-07  2.68778E-07
         5
.93272
E
-07  end
end
 response

r
e
s
p
o
n
s
e 4

t
i
t
l
e
=
"
t
o
```

(continues on next page)

(continued from previous page)

```
p
h
o
t
o
n

v
a
l
u
e
s 11
r1
.0  8
r0
.0 end
end
 response

r
e
s
p
o
n
s
e 99

t
i
t
l
e
=
"
p
u
t
a 1
i
n
e
v
e
r
y
g
r
o
u
p
"

n
e
u
t
r
o
n
```

(continues on next page)

(continued from previous page)

```
u
n
i
t
y
end
 response
```

The different response types all share some optional keywords. The keyword "makeChart" can be used to produce a *.chart file (called '*outputName*.resp*id*.chart') so that the response can be plotted with the ChartPlot 2D plotter. To create files for every response, use the keyword "makeCharts" inside the definitions block but outside any particular response definition. The keyword "multiplier=" can be used with any type of response, which is useful for things such as units conversions. Multiple uses of the "multiplier=" keyword within one response definition will apply the product of all multipliers to that response. Using the keyword "multiplier=" in the definitions block but outside any particular response will apply that multiplier to all responses. Keywords "eHigh=" and "eLow=" can be used to only keep the response values in a range between eHigh and eLow (both in eV). The keyword "lessOutput" can be used to suppress response data echoing in the output file and minimize output file size particularly for CE responses that can have fine point-wise data. It will cause to print only the first five and the last five points of the data if the number of bins is greater than twenty for binned histogram and value/function pairs type of responses.

The original flux-to-dose conversion factor references that were incorporated into Monaco are:

- ANSI/ANS-6.1.1-1977 (N666) "American National Standard Neutron and Gamma-Ray Flux-to-Dose-Rate Factors," Prepared by the American Nuclear Society Standards Committee Working Group ANS-6.1.1, Published by the American Nuclear Society, 555 North Kensington Avenue LaGrange Park, Illinois 60525, Approved March 17, 1977 by the American National Standards Institute, Inc.
- ANSI/ANS·6.1.1-1991, "American National Standard for Neutron and Gamma-Ray Fluence-to-Dose Factors," Prepared by the American Nuclear Society Standards Committee Working Group ANS-6.1.1, Published by the American Nuclear Society, 555 North Kensington Avenue LaGrange Park, Illinois 60525 USA, Approved August 26, 1991 by the American National Standards Institute, Inc.
- H. C. Claiborne and D. K. Trubey, "Dose Rates in a Slab Phantom from Monoenergetic Gamma Rays," *Nuclear Applications & Technology*, Vol. 8, May 1970.
- B. J. Henderson, "Conversion of Neutron or Gamma Ray Flux to Absorbed Dose Rate," ORNL Report No. XDC-59-8-179, August 14, 1959.
- International Commission of Radiation Units and Measurements, *ICRU Report 44: Tissue Substitutes in Radiation Dosimetry and Measurement*, Bethesda, MD, 1989.
- International Commission of Radiation Units and Measurements, *ICRU Report 57: Conversion Coefficients for use in Radiological Protection Against External Radiation*, Bethesda, MD, August 1, 1998.

Grid geometries

Grid geometries ("gridGeometry") require an identification number and then a description of a 3-D rectangular mesh by specifying the bounding planes of the cells in each of the x, y, and z dimensions. The keyword "xplanes … end" can be used to list plane values (in any order). The keyword "xLinear *n a b*" can be used to specify n cells between a and b. The keywords "xplanes" and "xLinear" can be used together and multiple times – they will simply add planes to any already defined for that dimension. Any duplicate planes will be removed. Similar keywords are used for the y- and z-dimensions.

```
g
r
i
d
G
e
o
m
e
t
r
y 3

t
i
t
l
e
="Boring uniform grid"

x
L
i
n
e
a
r 10
-100 100

y
L
i
n
e
a
r 10
-100 100

z
L
i
n
e
a
r 10
-100 100
end
 gridGeometry

g
r
i
d
G
e
o
m
```

(continues on next page)

```
e
t
r
y 2
```

(continued from previous page)

```
x
p
l
a
n
e
s
-100
.0
-90
.0
-99
.0
-95
.0 end

x
L
i
n
e
a
r  9
-90
.0  0
.0

x
L
i
n
e
a
r 18   0
.0 90
.0

x
p
l
a
n
e
s 95
.0 100
.0 99
.0  end

y
L
i
n
e
a
r 20  100
.0
```

(continues on next page)

```
-100
.0
```

(continued from previous page)

```
z
L
i
n
e
a
r 40  100
.0
-100
.0
end
 gridGeometry
```

When using multiple instances of the keyword *Linear and *planes for a given dimension, duplicates should be removed from the final list. In some cases, double precision math will leave two planes that are nearly identical but not removed (for example: 6.0 and 5.9999999). To prevent this, a default tolerance is set to remove planes that are within 10^{-6} cm of each other. The user is free to change this by using the keyword "tolerance=" and specifying something else. Note that the tolerance can be reset to a different value in between each use of *Linear or *planes.

The keyword "make3dmap" for a particular grid geometry definition will create a file called '*outputName*.grid*id*.3dmap' which can be visualized using the Java Mesh File Viewer. Using the keyword "make3dmaps" in the definitions block but outside any particular gridGeometry definition will create a geometry file for each gridGeometry defined.

Cylindrical mesh geometries

Cylindrical geometries ("cylGeometry") require an identification number and then a description of a 3-D cylindrical mesh by specifying the bounding planes of the cells in each of the *r*, , and *z* dimensions. The keywords "radii . . . end", "thetas . . . end", and "zplanes . . . end" can be used to list the plane values in any order. The keywords "radiusLinear *n a b*", "thetaLinear *n a b*", and "zLinear *n a b*" can be used to specify *n* cells between *a* and *b*. Note that the keywords "thetas" and "thetaLinear" expect values between 0 and 2. For entering values between 0 and 360°, use the keywords "degrees" and "degreeLinear" instead. The keywords for each dimension can be used together and multiple times – they will simply add planes to any already defined for that dimension. Any duplicate planes will be removed.

Cylindrical meshes are oriented along the positive z-axis by default. To change this, the user can specify the axis of the cylinder using the keyword "zaxis *u v w*" and specify the perpendicular direction where =0 using "xaxis *u v w*". To change the base position of the cylinder, use the keyword "position *x y z*". Some examples of cylindrical mesh geometries include:

```
c
y
l
G
e
o
m
e
t
r
y 12

r
a
d
i
u
s
L
i
n
e
```

(continues on next page)

(continued from previous page)

```
r
a
d
i
u
s
L
i
n
e
a
r 10 168
.0 368
.0

d
e
g
r
e
e
L
i
n
e
a
r 12 0 360

z
L
i
n
e
a
r 25 255
.2
-255
.2

z
P
l
a
n
e
s
-45
.0
-40
.
-35
.0 end
end
 cylGeometry

c
y
l
G
e
o
m
e
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="degenerate: only one angular bin"

r
a
d
i
u
s
L
i
n
e
a
r 10 168
.0 368
.0

t
h
e
t
a
L
i
n
e
a
r  1 0
.0 6
.2831853

z
L
i
n
e
a
r 25 255
.2
-255
.2
end
 cylGeometry

c
y
l
G
e
o
m
e
t
r
y 14
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="degenerate: emulate surface tally over partial angle range"

r
a
d
i
u
s
L
i
n
e
a
r 1 367
.5 368
.5

d
e
g
r
e
e
L
i
n
e
a
r 1 45 135

z
L
i
n
e
a
r 25 255
.2
-255
.2

z
a
x
i
s 0 0 1

x
a
x
i
s 0
-1 0
```

(continues on next page)

(continued from previous page)

```
end
cylGeometry
```

Similar to the grid geometries, the user can use the keyword "tolerance=" to specify how close duplicate planes can be when being considered for removal. The keyword "makeCylMap" for a particular cylindrical geometry definition will create a file called '*outputName*.cyl*id*.3dmap' which can be visualized using the Java Mesh File Viewer. Using the keyword "makeCylMaps" in the definitions block but outside any particular gridGeometry definition will create a geometry file for each gridGeometry defined. The Mesh File Viewer is written for rectilinear geometries and will not display circles. The only view that works in the Mesh File Viewer for cylindrical meshes is the *x*-*z* view, which will correctly show an *r*-*z* slice. The slider (marked "*y*") will control which value to display (from 0 to 2).

Cylindrical meshes can only be used for tallies. They cannot be used for making mesh sources or for any importance calculations in MAVRIC.

Distributions

Distributions ("distribution") require an identification number and several other keywords depending on the type of distribution. For a binned histogram distribution over *n* intervals, the keyword "abscissa ... end" is used to list the $n + 1$ bin boundaries and the keyword "truePDF ... end" is used to list the n values of the pdf integrated over those bins. For a pdf defined using a series of evaluated points over n intervals, use the keywords "abscissa ... end" and "truePDF ... end" listing the $n + 1$ values for each. The "truePDF" values should be the value of the pdf evaluated at the corresponding point in the abscissa array. The abscissa array should either be in increasing order or decreasing order – monotonic either way – with the truePDF array ordered accordingly.

For either the binned histogram or the value/function point pairs distributions, biasing can also be specified for a given distribution using the "biasedPDF ... end" keyword, the "weight ... end" keyword, or the "importance ... end" keyword, with a length that matches the truePDF array. Weights specify the suggested sampling weights for particles and importances specify the suggested importance. For biasing, the user only needs to specify just one of "biasedPDF", "weight" or "importance". The other arrays will be computed by Monaco.

For discrete distributions (such as gamma line sources), use the keyword "discrete ... end" to list the discrete abscissa values and use the keyword "truePDF ... end" to list the probabilities. The "biasedPDF ... end", "trueCDF ... end", and "biasedCDF ... end" keywords can also be used. Each array should have the same length – the number of discrete lines.

To visualize a distribution, add the keyword "runSampleTest" and a *.chart file will be produced showing the true pdf, the pdf used for sampling (the biased pdf) and the results of a sampling test using 10^6 samples. The file will be named using the output name of the SCALE job and the distribution identification number '*outputName*.dist*id*.chart' and can be viewed with the ChartPlot 2D Interactive Plotter. To perform a sampling test and create a *.chart file for all of the distributions in the definitions block, use the keyword "runSampleTests" inside the definitions block but outside any particular distribution.

Some example distribution inputs are listed below and shown in Fig. 5.12.

```
d
i
s
t
r
i
b
u
t
i
o
n 11
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="a binned histogram"

a
b
s
c
i
s
s
a
-5
-4
-3
-2
-1 0 1 2 3 4 5 end

t
r
u
e
P
D
F   1  2  3  4  5 4 3 2 2 2   end
end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 12

t
i
t
l
e
="value/function pairs"

a
b
s
c
i
s
s
a
-5
-4
-3
-2
-1 0 1 2 3 4 5 end
```

(continues on next page)

(continued from previous page)

```
t
r
u
e
P
D
F     0  1  2  3  4 5 4 3 2 2 2  end
end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 21

t
i
t
l
e
="a binned histogram with biasing"

a
b
s
c
i
s
s
a
-5
-4
-3
-2
-1 0 1 2 3 4 5 end

t
r
u
e
P
D
F   1  2  3  4  5 4 3 2 2 2   end

b
i
a
s
e
d
P
D
F 3  2  1  1  1 1 1 2 2 2   end
```

(continues on next page)

(continued from previous page)

```
end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 22

t
i
t
l
e
="value/function pairs with importances"

a
b
s
c
i
s
s
a
-5
-4
-3
-2
-1 0 1 2 3 4 5  end

t
r
u
e
P
D
F     0  1  2  3  4 5 4 3 2 2 2  end

i
m
p
o
r
t
a
n
c
e  4  3  2  1  1 1 1 1 2 2 2  end
end
 distribution
```

(continues on next page)

(continued from previous page)

```
d
i
s
t
r
i
b
u
t
i
o
n 31

t
i
t
l
e
="a binned histogram using CDF's"

a
b
s
c
i
s
s
a
-5
-4
-3
-2
-1  0  1  2  3  4 5 end

t
r
u
e
C
D
F   1  3  6 10 15 19 22 24 26 28   end
end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 32
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="a binned histogram with biasing using CDF's"

a
b
s
c
i
s
s
a
-5
-4
-3
-2
-1  0  1  2  3  4 5 end

t
r
u
e
C
D
F   1  3  6 10 15 19 22 24 26 28   end

b
i
a
s
e
d
P
D
F 3  5  6  7  8  9 10 12 14 16   end
end
 distribution
```

Other notes on distributions:

1) Binned histogram distributions can also be specified using cdf's (keywords "trueCDF" and "biasedCDF").

2) For distributions that will be used for source energy sampling, use abscissa values of eV.

3) For multigroup calculations using histograms, the keywords "neutronGroups" or "photonGroups" can be used instead of specifying the abscissa values. In this case, be sure to list the binned pdf values in order from the highest energy group to the lowest energy group.

4) For CE calculations, instead of specifying abscissa values, the bin boundaries of an energyBounds object (see next section) can be specified using "energyBoundsID=".

Several special (built-in) distributions are available in Monaco. To use one of these, specify the keyword "special=" with a distribution name in quotes and the keyword "parameters ... end" (if required) for that type of distribution. These special distributions are summarized in Table 8.2.8.

Fig. 5.12: Sampling tests for the distribution examples.

The Watt spectrum has the form

$$p(E) = ce^{-E/a}\sinh(\sqrt{bE}) \tag{5.18}$$

with the parameters *a* and *b* (with *c* as a normalization constant). For spontaneous fission of ^{252}Cf, values typically used are *a*=1.025 MeV and *b*=2.926/MeV. For thermal fission of ^{235}U, the parameters are *a*=1.028 MeV and *b*=2.249/MeV. For induced fission, the parameters *a* and *b* are, in general, functions of incident neutron energy. See Table 8.2.9 for an example. The Watt spectrum distribution will be displayed in the *.chart plot as a histogram distribution using the cross-section energy structure neutron groups but when sampled in Monaco, the continuous Froehner and Spencer[1] method is used to select an energy of source particles using a Watt spectrum distribution.

with the parameters *a* and *b* (with *c* as a normalization constant). For spontaneous fission of ^{252}Cf, values typically used are *a*=1.025 MeV and *b*=2.926/MeV. For thermal fission of ^{235}U, the parameters are *a*=1.028 MeV and *b*=2.249/MeV. For induced fission, the parameters *a* and *b* are, in general, functions of incident neutron energy. See Table 8.2.9 for an example. The Watt spectrum distribution will be displayed in the *.chart plot as a histogram distribution using the cross-section energy structure neutron groups but when sampled in Monaco, the continuous Froehner and Spencer[1] method is used to select an energy of source particles using a Watt spectrum distribution.

Table 5.8: Special (built-in) distributions

Distribution	Parameters	Description
"wattSpectrum"	*a b n*	Watt spectrum distribution. Units are: *a* in MeV, *b* in /MeV. Optional parameter *n* specifies how many subintervals in each neutron group to use in integrating the pdf (default 100) for the histogram representation in the sampling test and mesh source representation.
"fissionNeutrons"	*m ZAID*	Spectrum of fission neutrons from the MULTIGROUP cross-section library for material *m* and nuclide *ZAID*.
"fissionPhotons"	*ZAID*	Spectrum of fission photons from nuclide *ZAID*.
"origensBinaryConcent rationFile"	*c s*	Spectrum from an ORIGEN-S binary concentration file case number *c*, spectra type *s*. For the spectra type *s*, values are: 1 – total neutron, 2 – spontaneous fission, 3 – (,n), and 4 – delayed neutrons, 5 – photons. The ORIGEN-S filename should be supplied with the keyword filename= "…" and the path/filename in quotes.
"cosine"	*n*	Cosine function from – /2 to /2. Optional parameter *n* (default 100) is the number of value/function pairs to show in the sampling test.
"pwrNeutronAxialProfi le"	none	Typical neutron PWR axial profile.
"pwrGammaAxialProfile"	none	Typical gamma PWR axial profile.
"pwrNeutronAxialProfi leReverse"	none	Typical neutron PWR axial profile, reversed top to bottom.
"pwrGammaAxialProfile Reverse"	none	Typical gamma PWR axial profile, reversed top to bottom.
"exponential"	*a n*	Exponential function *eax* from -1 to 1. Optional parameter *n* (default 100) is the number of value/function pairs to show in the sampling test.
"origensDiscreteGammas"	*z a m*	Discrete gammas from the ORIGEN mpdkxgam database for isotope of atomic number *z*, mass *a* and metastable state *m*. (default is m=0)

For the ORIGEN-S binary concentration sources, the ORIGEN input file should be specified using the filename="…" with the path/filename in quotes. Note that the ORIGEN calculation has to be set to save the neutron or photon data will be used as a Monaco distribution. This can be done by specifying the number of photon or neutron groups on the 3$ (library integer constants) array and specifying the energy bin boundaries on the 83* and 84* (group structure) arrays. In Monaco, to show all of the cases in the binary concentration file, ask for case 0. To show what data is available for a particular case, ask for that case number and spectra type 0.

Other notes on special distributions: 1) Fission neutron distributions use MT=1018 for the specified ZAID of the specified isotope from the cross-section library. 2) Fission photon distributions are not read from the cross-section file but are instead read from a separate file containing only ENDF/B-VII.0 fission photon data. 3) The neutron and photon

axial profile distributions come from the SCALE 5.1 SAS4 manual, Table S4.4.5. 4) Fission neutron distributions are not allowed in the CE problems, users are advised to use "wattSpectum" in order to get a similar distribution.

Table 5.9: Watt spectrum parameters for neutron induced fission of ^{233}U (From ENDF/B-VII.0)

Energy (MeV)	a (MeV)	b (/MeV)
1.E-11	0.977	2.546
1.5	0.977	2.546
2	0.980	2.532
5	1.010	2.412
7	0.970	2.571
10	0.980	2.474
12.2	1.010	2.612
15	1.000	2.652
18	1.040	2.689
20	1.060	2.620
30	1.060	2.620

Some example special distribution inputs are listed below and shown in Fig. 5.13.

```
d
i
s
t
r
i
b
u
t
i
o
n 11

s
p
e
c
i
a
l
="wattSpectrum"

p
a
r
a
m
e
t
e
r
s 1
```

(continues on next page)

(continued from previous page)

```
end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 12

s
p
e
c
i
a
l
="fissionNeutrons"

p
a
r
a
m
e
t
e
r
s 1 92235 end
end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 21

s
p
e
c
i
a
l
="fissionPhotons"
```

(continues on next page)

(continued from previous page)

```
p
a
r
a
m
e
t
e
r
s 94239 end
end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 22

s
p
e
c
i
a
l
="origensBinaryConcentrationFile"

f
i
l
e
n
a
m
e
="c:\\path\somefile.f71"

p
a
r
a
m
e
t
e
r
s 9 5 end
end
 distribution
```

(continues on next page)

(continued from previous page)

```
d
i
s
t
r
i
b
u
t
i
o
n 31

s
p
e
c
i
a
l
="origensBinaryConcentrationFile"

f
i
l
e
n
a
m
e
="c:\\path\somefile.f71"

p
a
r
a
m
e
t
e
r
s 9 1 end
end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 32
```

(continues on next page)

(continued from previous page)

```
s
p
e
c
i
a
l
="cosine"

p
a
r
a
m
e
t
e
r
s 100 end
end
 distribution

d
i
s
t
r
i
b
u
t
i
o
n 41

s
p
e
c
i
a
l
="pwrNeutronAxialProfile"
end
 distribution

d
i
s
t
r
i
b
u
t
i
```

(continues on next page)

```
o
n 42
```

(continued from previous page)

```
s
p
e
c
i
a
l
="exponential"

p
a
r
a
m
e
t
e
r
s 1
.0 100 end
end
 distribution
```

Energy boundaries

Energy boundaries ("energyBounds") require an identification number and a specification of a set of bin boundaries in energy (eV). Energy bounds objects are typically used in CE calculations for specifying and energy grid for tallies. The keyword "bounds … end" can be used to list energy values (in eV, in any order). The keyword "linear *n a b*" can be used to specify *n* bins between *a* and *b*. Likewise, the keyword "logarithmic *n a b*" can be used for n bins logarithmically spaced between *a* and *b*. The keywords "bounds", "linear" and "logarithmic" can be used together and multiple times – they will simply add energy boundaries to any already defined. Any duplicate planes will be removed using the absolute tolerance, specified with the keyword "tolerance=". To specify one of the more common SCALE energy structures (handy for doing tallies one a standard structure in CE calculations), one of the following shortcut keywords can be used: "252n", "238n", "200n", "56n", "47p", "44n", "27n", or "19p".

These keywords will cause to load the energy structures from the MG cross-section libraries aliased in the "FileNameAliases.txt" with names of "xn252", "xn238", "xn200", "xn56", "xg47", "xn44", "xn27", and "xg19" relatively. If required energy structure is for neutrons and there is no alias for MG cross-section library or the library is missing, MG JEFF reaction data library will be searched as "n{NG}.reaction.data" to load the energy structure. These can be used in combination with the other keywords to use existing structures supplemented with extra boundaries.

```
e
n
e
r
g
y
B
o
u
n
d
s 1
```

(continues on next page)

Fig. 5.13: Sampling tests for the special (built-in) distribution examples.

(continued from previous page)

```
t
i
t
l
e
="bounds command, check for duplicates"

b
o
u
n
d
s 1 4 2 3 5 end

b
o
u
n
d
s 7 6 10 5 9 8 7 end
end
 energyBounds

e
n
e
r
g
y
B
o
u
n
d
s 3

t
i
t
l
e
="logarithmic command"

l
o
g
a
r
i
t
h
m
i
c  21  1
.0 10000000
.0
```

(continues on next page)

(continued from previous page)

```
end
 energyBounds

e
n
e
r
g
y
B
o
u
n
d
s 11

t
i
t
l
e
="SCALE 19 group photon structure with extras"
    19
p

l
i
n
e
a
r 10 6
.0
e6 7.0e6
end
 energyBounds
```

An energyBounds object can also be used to set the energy bin boundaries for a response (type1) instead of using the "bounds … end" keyword. This is done by using with the keyword "energyBoundsID=" and referencing a defined energyBounds object. Likewise for distributions, instead of specifying the "abscissa … end" keyword and listing abscissa values, an energyBounds object can be used. This allows the user to define a set of energy bin boundaries once and re-use them across multiple responses and definitions. When using the "energyBoundsID=" keyword, the data values should be entered in the standard multigroup order – from high energy to low energy. For a stand-alone multigroup Monaco calculation, do not use ID numbers of 1 or 2 for energyBounds objects – these ID numbers are reserved.

Time boundaries

Time boundaries ("timeBounds") are similar to energy bin boundaries but take values in seconds. These objects are only used in tallies in CE calculations.

```
t
i
m
e
B
o
u
n
d
s 2

t
i
t
l
e
="linear command"

l
i
n
e
a
r 10 0
.0 10.0e-3
end
 timeBounds

t
i
m
e
B
o
u
n
d
s 7

t
i
t
l
e
="logarithmic command"

l
o
g
a
r
i
t
h
m
i
c  6  1
.0
e
-6 1
.0
```

(continues on next page)

(continued from previous page)

```
end
 timeBounds
```

5.3.5 Sources block

The sources block specifies what sources to use. Multiple sources are allowed and each is sampled according to its strength, relative to the total strength of all sources. Each source description must be contained with a "src *id*" and an "end src" (where the *id* is the source identification number). The sources block must contain at least one source.

For each user-defined source, the user can specify the spatial distribution, the energy distribution and the directional distribution separately. Many options for each distribution are available and defaults are used for most if the user does not specify anything. The source strength is set using the keyword "strength=" and the type of source is set using the keyword "neutron" or "photon". The "strength=" keyword is required for each source.

When using more than one source, the user can set the true strength of each using the keyword "strength=" and can also specify how often to sample each source using the keyword "biasedStrength=". The true strengths of the sources will be combined to form the true source distribution PDF. The biased strengths of sources will be combined to form a PDF from which to sample. The weights of the source particles will be properly weighted to account for the biased sampling strengths. For example, consider two sources of strengths 10^9 and 9×10^9 /sec that should be sampled in a ratio of 4:1. The biased sampling strengths are then set to 4 and 1. Monaco will sample the first source 80% of the time and the particles will be born with a weight of 0.125. The second source will be sampled 20% of the time and its particles will be born with weights of 4.5.

Spatial distribution

Keyword	Parameters	Possible degenerate cases
cuboid	x_{max} x_{min} y_{max} y_{min} z_{max} z_{min}	rectangular plane, line, point
xCylinder	*r* x_{max} x_{min}	circular plane, line, point
yCylinder	*r* y_{max} y_{min}	circular plane, line, point
zCylinder	*r* z_{max} z_{min}	circular plane, line, point
xShellCylinder	*r1 r2* x_{max} x_{min}	cyl., planar annulus, cyl. surface, line, ring, point
yShellCylinder	*r1 r2* y_{max} y_{min}	cyl., planar annulus, cyl. surface, line, ring, point
zShellCylinder	*r1 r2* z_{max} z_{min}	cyl., planar annulus, cyl. surface, line, ring, point
sphere	*r*	point
shellSphere	*r1 r2*	sphere, spherical surface, point

Note that other than the shell-type solids, the parameters are the same as the SGGP geometry specification of those solids. The SGGP keyword "origin" (followed by at least one of "x=", "y=", and/or"z=") is available for all of the different source solid bodies. For the cylinder based solid bodies, the direction of the axis of the cylinder can be set by using the keyword "cylinderAxis *u v w*", where *u*, *v*, and *w* are the direction cosines with respect to the global *x*-, *y*-, and *z*-directions.

The source can be limited to only be from the parts of the solid body that are inside a specific unit ("unit="), inside a specific region ("region=") within the specified unit, or made of a certain material ("mixture="). A mixture and a unit/region cannot both be specified since that would either be redundant or mutually exclusive.

If no source spatial information is provided by the user, the default is a point source located at the origin (in global coordinates). Like SGGP input, the geometry keywords used for the bounding shape are fixed lengths arrays and do not have an "end" terminator. They must be followed by the correct number of parameters.

The spatial distribution in each dimension of the cuboid shape is specified by using the keywords "xDistributionID=", "yDistributionID=", or "zDistributionID=" and pointing to a distribution defined in the definitions block. For the

cylindrical shapes, "rDistributionID=" and "zDistributionID=" can be used. For spherical shapes, only the "rDistributionID=" can be specified. Distributions defined using abscissa values that are different than the length of the simple geometry bounding shape can still be used if the keyword "xScaleDist" (or "y", "z", or "r") is used. This linearly scales the distribution abscissa values to the length of the simple geometry bounding shape. Note that for cylindrical sources, since the axis can point in any direction, the z distribution is interpreted as the length along the axis, with the base position as z=0.

Energy distribution

"eDistributionID=" and pointing to one of the distributions defined in the definitions block. Energies will be sampled from the distribution in a continuous manner. For MULTIGROUP calculations, that energy will then be mapped onto the group structure of the cross-section library being used by Monaco. Each source should have an energy distribution that has abscissa values in units of eV. If no energy distribution is given, 1 MeV (translated to the current group structure if a multigroup problem) will be used.

To use the total of an energy distribution as the source strength, use the keyword "useNormConst" without either "strength=" or "fissions=". This will set the strength to be equal to the normalization constant of the distribution – the total of the distribution before it was normalized into a pdf. An optional "multiplier=" keyword can be used to increase or decrease that strength. For example, consider a case using the neutron spectrum information from a case of an ORIGEN-S binary concentration file that used a basis of an entire core. If the Monaco source was just one of the 200 assemblies, then the "multiplier=" keyword can be set to 0.005 so that the source strength is scaled appropriately.

Directional distribution

The directional distribution of the source is specified by using the keyword "dDistributionID=" and pointing to one of the distributions defined in the definitions block. The distribution will be used to sample the cosine of the polar angle, μ, from the reference direction. The reference direction, where $\mu = 1$, is set with the keyword "direction *u v w*", where *u*, *v*, and *w* are the direction cosines with respect to the global *x*-, *y*-, and *z*-directions. The default value for the reference direction is the positive *z*-axis (<0,0,1>). The keyword "dScaleDist" can be used to linearly scale the distribution abscissa values to the range of $\mu \in [-1, 1]$. If no directional distribution is specified with the keyword "dDistributionID=", then an isotropic directional distribution will be used.

Using a Monaco mesh source map file

The user can alternatively specify an existing Monaco mesh source map file—a binary file created by a previous MAVRIC or Monaco calculation. The mesh source map must be a binary file using the Monaco mesh source map format (a *.msm file). This option is specified with the "meshSourceFile=" keyword and the file name (and full path if necessary) in quotes.

```
read
 sources

s
r
c 1

m
e
s
h
S
o
u
r
c
e
F
i
l
e
=
```

(continues on next page)

(continued from previous page)

```
    end
 src
end
 sources
```

If the "meshSourceFile=" keyword is used, all energy distribution keywords and most spatial distribution keywords will be ignored. Source keywords that can be used with a mesh source include "strength=" to override the source strength in the mesh source; "biasedStrength=" to set the sampling strength; "origin", "x=", "y=", and "z=" to place the origin of the mesh source file at a particular place in the current global coordinate system; and the keywords for describing the directional distribution – "dDistributionID=", "direction *u v w*" and "dScaleDist".

Mesh sources are sampled using the following algorithm: First, a direction is sampled. Second, a voxel is sampled and a position is picked uniformly within the voxel. If that position does not match the optional limiters (unit, region, material specified in the mesh source), a new position is chosen within the voxel until a match is made. If a position cannot be found within the voxel after 10000 tries, Monaco will stop. (This can occur if the mesh voxel contained just a sliver of source volume when generated. For this case, the keyword "allowResampling" can be used to select a new voxel instead of stopping. In general, this keyword should not be used.)

Creating a mesh source

To create a mesh source out of the source definition, use the "meshSourceSaver" subblock inside the sources block. It is quite handy to visualize the sources and ensure they are what were intended. You must specify which one of the defined grid geometries to use (keyword "gridGeometryID=") and a filename for the resulting mesh source file (keyword "filename=" with the filename in quotes "*path\name*.msm"). For more than one source, each will be stored separately and the filename will include the source id number.

```
read
 sources

s
r
c 1

...

...
    end
 src

s
r
c 5

...

...
    end
 src

m
e
s
h
S
o
u
r
c
e
S
a
v
```

(continues on next page)

(continued from previous page)

```
g
r
i
d
G
e
o
m
e
t
r
y
I
D
=7

f
i
l
e
n
a
m
e
="meshSource.msm"

s
u
b
c
e
l
l
s
=3
    end
 meshSourceSaver
end
 sources
```

To create the mesh source, Monaco determines if the defined source exists within each cell. This is done by dividing each mesh cell into $n \times n \times n$ subcells (from the keyword subCells=n with a default of n=2) and testing each subcell center. For every subcell center that is a valid source position (within the spatial solid and meets the optional unit, region, or mixture requirements), an amount of source proportional to the subcell volume is assigned to the mesh cell. The keyword subCells= can be used to better refine how much source is computed for the mesh cells at the boundary of a curved source region. Of course, more subcell testing takes more time. If a given source is degenerate in any dimension (point, line, or plane), that information will be stored in the resulting mesh source so that particles will not be sampled over the entire corresponding voxel but will have closer to the original spatial distribution. Likewise, if the original source had restrictions based on unit, region or mixture, those restrictions will be stored as part of the resulting mesh source.

The above process may miss small sources or degenerate sources (surfaces, lines, points) that do not lay on the tested subcell centers. If none of the mesh cells contain any source after the subcell method, then random sampling of the source is used. A number of source positions are sampled from the source (set by the "sourceTrials=" keyword, default of 1000000) and then placed into the proper mesh cell. If this method is used, the resulting mesh source file should be

visualized to ensure that the statistical nature of the source trials method does not unduly influence the overall mesh source. To skip the subcell method and go directly to the source trials method, use "subCells=0".

The keyword "makeTotal" will make a single mesh source file which is the composite of all of the individual sources. Geometric degeneracies or restrictions to only sample particles from a specified unit, region or material will only be kept if they are the same for all of the sources. For this reason, users may not wish to use a mesh source using the "makeTotal" keyword for transport but rather use it to verify that all of the sources have been input properly.

The keyword "reduce" can be used to only save the smallest rectangular portion of the mesh surrounding the voxels with non-zero source amounts. This can result in much smaller file sizes for sources that are small compared to the extents of the grid geometry.

Monaco mesh source files (*.msm) can be viewed with the Mesh File Viewer. Plots can be made showing the source values for each group (or total). The viewer can also show the geometry regions or material mixtures as well. Using the viewer is an easy way to confirm that the source definition was entered correctly. Note that the *.msm files actually only store the biased sampling distribution and the initial weights (to speed up the sampling process). So, in the viewer the "true" source is computed as the product of the sampled distribution and the weights. If groups with real source are set to zero importance, the viewer cannot recreate the original true source. The true source shown by the viewer is the amount of true source only in groups that have non-zero importance.

Mesh source advanced features

Two advanced features exist in the meshSourceSaver subblock – mainly used by the MAVRIC sequence when the importance map calculations use a different cross-section library than the final Monaco calculation.

The keyword "sampleFromMesh" can be used to tell Monaco to sample from the created mesh file(s) instead of the standard source definition. This can be useful in determining if the mesh source is fine enough to accurately represent the original source definition. If the "makeTotal" keyword was used, then Monaco will sample from the total mesh source file.

The keyword "meshBiasFile=" can be optionally be used when "sampleFromMesh" is on. This tells Monaco to sample from the mesh source file(s) version of the source definition that has been modified using just the importance information from the named mesh source file. For example, using a 27-group biased mesh source for a Watt spectrum source may not represent the high energy tail very well. In this case, it would be better to do a 200-group Monaco calculation but still use the importance information from 27-group mesh source file using "sampleFromMesh" and "meshBiasFile=".

5.3.6 Tallies block

The tallies block tells Monaco what to compute: fluxes at certain points in space (point detectors), fluxes in certain geometry regions, or fluxes in each voxel of a mesh grid. The computed fluxes can also be integrated with response functions to compute dose, reaction rate or some other dose-like quantity. Any number of optional response functions can be evaluated with each tally.

Each tally type begins with a keyword ("pointDetector", "regionTally", or "meshTally") and ends with an "end" and that same keyword. Individual tallies can be listed in any order. Identification numbers for each tally are required and must be positive integers and unique among the tally type. All three of the tally types can have an optional title using the keyword "title=" followed by the title enclosed in double quotes. Tallies should be defined as either a neutron tally or a photon tally.

```
read
 tallies

p
o
i
n
t
D
e
t
e
c
```

(continues on next page)

(continued from previous page)

```
...
    end
 pointDetector

r
e
g
i
o
n
T
a
l
l
y 9

...
    end
 regionTally

r
e
g
i
o
n
T
a
l
l
y 19

...
    end
 regionTally

m
e
s
h
T
a
l
l
y 1

...
    end
 meshTally
end
 tallies
```

Each tally computes the fluxes in each tally bin and the total flux. For multigroup calculations, the multigroup cross section group structure is used for all tallies. For CE calculations, each tally can use a different "energyBoundsID=", which points to one of the energy bounds defined in the definitions block. CE calculations can also use the keyword "timeBoundsID=" to specify a set of time bin boundaries. For one response function to integrate the fluxes with, the

keyword "responseID=" can be used, where the value corresponds to the identification number of one of the response functions defined in the definitions block. For multiple response functions, the keyword array "responseIDs … end" can be used.

Each tally type can be multiplied by using the "multiplier=" keyword. This is useful for units conversions or other types of scaling. Multiple uses of the multiplier keyword within one tally definition will apply the product of all multipliers to that tally. Using the keyword "multiplier=" inside the tallies block but outside any particular tally will apply that multiplier to all tallies.

Point detector tallies

A point detector tally computes the uncollided and total flux at a given location in space. This tally requires exactly one location and can use any number of optional response functions. The "locationID=" keyword is used to specify one of the locations listed in the definitions block. Point detectors should only use locations that are in void regions of the geometry.

Because point detectors estimate the flux at the location using a ray-trace from every collision site during the life of the particle, they can be quite expensive. For particles very far away from the detector location, the contributions to the tally can be quite small. Point detectors can be made to use the importance of the current particle location/energy to decide whether or not to make a contribution to the tally using the keyword "minSampProb=" and a value such as 0.1 or 0.01. This keyword specifies the minimum sampling probability for a given point detector. As the particle is transported, the probability p of making a contribution to the point detector tally is set by using the current weight of the particle, w, to be

$$p = \left(\frac{w_{\min}}{w}\right)^a \tag{5.19}$$

where the power a for each point detector was determined at the start of the simulation using the minimum sampling probability $p_{\min}$ to be

$$a = \frac{\ln\left(p_{\min}\right)}{\ln\left(\frac{w_{\min}}{w_{\max}}\right)} \tag{5.20}$$

where the minimum and maximum target weights, $w_{\min}$ and $w_{\min}$, were determined from either the region-based weight targets or the mesh-based importance map weight targets. So, when the current particle weight approaches the minimum target weight of the problem (in very important areas), the point detector contribution is made nearly 100% of the time. When the particle weight approaches the maximum target weight (in very unimportant areas), the contribution to the point detector tally is made with probability $p_{\min}$, saving quite a bit of computer time.

This option should only be used if the point detector location is in the area of high importance. For point detectors in areas of low importance, using this option may severely undersample the point detector where contributions would actually be the most significant, causing an underestimation of the flux. The default value for the minimum sampling probability is $p_{\min} = 1$, giving a default value of $a = 0$ so that the point detector contribution is made at every collision, independent of the current particle weight.

The keyword "minSampProb" used in the tallies block but outside any particular point detector tally specification will be applied to all point detectors.

Each point detector is summarized in the main output file. The uncollided and total flux for each particle type is listed as well as the values for the optional integrated response functions. Along with each of these quantities is a list of the standard deviation of the quantity, the relative uncertainty, the figure-of-merit and a summary of list of the statistical checks (passed or not). Group-by-group values of the fluxes and responses are listed in a separate file named "*outputName*.pd*id*.txt" where *outputName* is the name the user chose for his output file and "*id*" is the identification number corresponding to the point detector tally specification. This file also contains more information about the six statistical checks for flux and each response – their pass/fail values with each batch of simulated particles and their final numerical values at the end of the simulation. A second file called "*outputName*.pd*id*.chart" is also created which can be displayed using the ChartPlot 2D Interactive Plotter, to visually check the convergence behavior of the tally.

The total neutron flux, the total photon flux, and the total response function value for each response as a function of batch can be viewed.

Region tallies

A region tally computes both the track-length estimate and the collision density estimate of the flux over a given geometry region (an SGGP "media"). This tally uses the keywords "unit=", "region=", and "mixture=" to limit the tally to one or more of those aspects. For example, "unit=2" and "region=3" are used to specify a region tally for the 3rd media listed for unit 2 of the SGGP geometry input. A mixture and a unit/region cannot both be specified since that would either be redundant or mutually exclusive. If the volume of the region is not given (or calculated) in the SGGP input, then instead of flux, the tally will compute average track length and average collision density.

Each region tally is summarized in the main output file. The total flux for each particle type is listed as well as the values for the optional integrated response functions. Along with each of these quantities is a list of the standard deviation of the quantity, the relative uncertainty, the figure-of-merit and a summary of list of the statistical checks (passed or not). Group-by-group values of the fluxes and responses are listed in a separate file named "*outputName*.rt*id*.txt" where *outputName* is the name the user chose for his output file and "*id*" is the identification number corresponding to the region tally specification. This file also contains more information about the six statistical checks for flux and each response – their pass/fail values with each batch of simulated particles and their final numerical values at the end of the simulation. A second file called "*outputName*.rt*id*.chart" is also created which can be displayed using the ChartPlot 2D Interactive Plotter, to visually check the convergence behavior of the tally. The total neutron flux, the total photon flux, and the total response function value for each response as a function of batch can be viewed.

Mesh tallies

A mesh tally computes the track-length estimate of the flux for every cell in a grid (mesh) geometry. This tally requires exactly one grid geometry or cylindrical geometry and can use any number of optional response functions. The "gridGeometryID=" or "cylGeometryID=" keyword is used to specify one of the mesh geometries listed in the definitions block. The group-by-group flux values, the total flux values and the total for each response are kept in memory during the simulation. Group-by-group contributions to the responses are not tallied during the simulation.

Mesh tallies can be limited to only save contributions to the voxel flux from track lengths through a certain unit, region or material using the keywords "unit=", "region=", and "mixture=". For example, to compute a mesh tally of a reaction rate of a specific isotope, the response function should only be multiplied by the amount of flux in the voxel that resulted in contributions from the material that contained that isotope. In this case, the keyword "mixture=" should be used so that the fluxes in each voxel represent only the flux from that material that holds the desired isotope.

A mesh tally saves the flux for each group, as well as the integrated response functions for each listed response for every cell of the grid geometry to a file called "*outputName*.mt*id*.3dmap" where *outputName* is the name the user chose for his output file and "*id*" is the identification number corresponding to the mesh tally specification. This file contains the group flux values and their absolute uncertainties. If any response functions were specified, then the responses and their uncertainties will be computed and stored in the same file. Monaco mesh tally files can be viewed with the Mesh File Viewer.

With each mesh tally, files are also created with the statistical test information - "*outputName*.mt*id*.flux" and "*outputName*.mt*id*.resp*xx*.txt" where *xx* is the responseID. The statistical tests can be turned off with the keyword "noStatChecks".

The Mesh File Viewer can be used to show the value, uncertainty, or relative uncertainty of any of the group fluxes, total fluxes, or responses tallied. For characterizing the mesh tally, the viewer can be used to display histograms of the relative errors—showing what fraction of the mesh cells had less than some amount of relative uncertainty. Images from the Mesh File Viewer can be saved as *.jpg, *.bmp, *.gif or *.png files or exported to other applications, such as MS Word.

Mesh tally files can become quite large—if the group-by-group fluxes are not important for a given problem, the keyword "noGroupFluxes" can be added to the mesh tally input. Instead of the group fluxes, only the total neutron

and total photon fluxes will be written to the mesh tally file. If the group-by-group values for the response functions are required, the keyword "saveRespDetails" can be used to create separate mesh tally files of each response called "*outputName*.mt*id*.resp*id*.3dmap" where the second "*id*" is the response identification number. Note that for CE calculations, these group-by-group results are formed using the response function mapped onto the energy grid of the tally, since separate tallies of response by group are not made during the simulation.

The mesh tally keyword "weightless" will instruct Monaco to not include the particle weight in the contribution to the mesh tally for track lengths that cross the voxels of the mesh. Instead of a flux tally, this will compute the Monte Carlo particle density – a measure of the number of particles simulated by Monaco in each mesh cell and in each energy group.

Mesh tallies can use a cylindrical mesh instead of a rectilinear mesh. Use the keyword "cylGeometryID=" instead of "gridGeometryID=" and reference one of the defined cylindrical meshes defined in the definitions block. Both cannot be specified at the same time. The Java Mesh File Viewer can only show the *r*-*z* view of a cylindrical mesh tally.

5.3.7 Parameter Block

The parameter block sets the Monte Carlo parameters used by Monaco. Items can be listed in any order. The initial random number ("randomSeed=") is given as a 16-digit hexadecimal number. The number of histories per batch ("perBatch=") and the number of batches ("batches=") can be specified. After every batch of source particles, the tally files are saved to disk. To prevent long run times, a maximum run time in minutes ("maxMinutes=") can also be specified. Defaults are 10 batches of 1000 histories each, with no time limit. The value of batches is used to allocate arrays for the tally statistical tests – so do not make this overly large, even when using maxMinutes to control termination.

For MULTIGROUP, the particles contained in the library will be transported, unless turned off using the keywords "noNeutron" or "noPhoton." In CE, to prevent loading large amounts of unneeded cross-section information into memory, the user should specify which particles to transport, using the keywords "neutron" and/or "photon." Monaco also supports Doppler pre-broadening of the CE neutron cross sections. This is controlled by the "dopplerBroaden=" parameter. Integer options are 0 (disabled, default), 1 (broaden 1D cross sections only), 2 (broaden 1D and 2D cross sections), and 3 (broaden 2D cross sections normally and broaden 1D cross sections using a less robust, but faster, interpolation method).

The default behavior for Monaco is to create neutrons from fission events and create secondary gammas from neutron collisions. To turn off the creation of fission neutrons in all multiplying media (for example, when the source already includes them), use the keyword "fissionMult=0". For problems where the library has photon data but none of the tallies require photons, use the keyword "secondaryMult=0" to stop the creation of secondary photons from neutrons. In CE problems, the number of fission neutrons and secondary gammas can be simulated as one particle of each type having a high weight ("fissionMult=1", "secondaryMult=1") or as many particles as the physical yield for the reaction would dictate ("fissionMult=2", "secondaryMult=2"), each with a weight corresponding to their probability of emission. If the user requests option 2 and the particle bank becomes too large, Monaco will drop the settings back to option 1. In MULTIGROUP, values of 1 and 2 are both treated as 1.

```
read
 parameters

r
a
n
d
o
m
S
e
e
d
=003
e
c
d7
b4
e3
e8
```

(continues on next page)

(continued from previous page)

```
p
e
r
B
a
t
c
h
=100000
b
a
t
c
h
e
s
=100
m
a
x
M
i
n
u
t
e
s
=1440
.0

f
i
s
s
i
o
n
M
u
l
t
=0
end
 parameters
```

In complex geometries, particles can sometimes "get lost" due to round-off errors in the ray-tracing. This would normally result in the code stopping, since lost particles usually indicate an undefined or doubly defined region of space. In order to tolerate a few lost particles without stopping the code, use the keyword "maximumLost=". Care should be taken not to increase this just to get around poorly defined geometry. To aid in geometry testing, the keyword "voidAllRegions" can be used. This keyword sets every region material to void so that tracks can stream through without interacting (faster). A large source and this keyword can be used to test a geometry input for gaps and overlaps. When the "voidAllRegions" keyword is used, mesh tally files will not contain material information, only the unit and region information.

Note that for both CE and MULTIGROUP, using fissionMult=0 only turns off the creation of neutrons from fission. The fission photons are controlled by the secondaryMult setting because some of the ENDF data evaluations do not

separate fission gammas from other neutron collision gammas.When using a mesh-based importance map, if a particle is outside the importance map, the code will stop with the message "Could not find particle importance. The particle is outside of the importance map." If the importance map does not cover the entire problem, then the tallies may be missing part of their final values. If the user intends to use an importance map that does not cover the entire geometry and wants particles outside the importance map to have zero importance (they will then be killed), then the keyword "allowShortImpMap" can be used to allow the use of a "short" importance map. Users must be sure that areas outside the importance map are unimportant to the problem.

5.3.8 Biasing Block

The optional biasing block lists the parameters for the standard Monaco variance reduction tools: forced collisions, region-based weight windows, and path-length stretching. This block also allows for the use of a previously made Monaco mesh importance map, such as those produced by the MAVRIC sequence.

Forced collisions

Forced collisions are one of the simplest variance reduction techniques. This makes a particle have a collision along its current flight direction before leaving the geometry. The collision is forced and the particle weight is reduced by the true probability of having a collision within the geometry. This is helpful in small or low-density geometries where many particles leave without interacting but can add computation time to ordinary problems. To use forced collisions, specify the "forcedCollisions" keyword. This requires the use of Russian roulette ("targetWeights" and "lowerWeights", see below).

Weight windows

Monaco can use Russian roulette for preventing low particle weights from being followed and splitting to prevent the production of very high weight particles. Either of these requires the target weight values ("targetWeights … end") for each energy group and for each region to be listed. For CE calculations, the energy bin boundaries are specified with the keywords "nEnergyBoundsID=" and "pEnergyBoundsID=". For Russian roulette, the lower weight bounds must be specified ("lowerWeights … end") and for splitting the upper weight bounds are listed ("upperWeights … end"). The different weight arrays can have a length matching (1) the product of the number of energy groups and the number of regions, (2) the number of regions, or (3) the number of energy groups. In case 2, the values are repeated for each energy group. In case 3, the values are repeated for each region. For example, to specify only Russian roulette in a coupled neutron-photon problem with target and lower weights the same in each region the following is used. An example using the 27/19 multigroup library would be

```
read
 biasing

t
a
r
g
e
t
W
e
i
g
h
t
s 27
r1
.0 19
r0
.1  end
```

(continues on next page)

(continued from previous page)

```
l
o
w
e
r
W
e
i
g
h
t
s  27
r0
.1 19
r0
.01 end
end
 biasing
```

and for a CE calculation

```
read
 definitions

e
n
e
r
g
y
B
o
u
n
d
s 1 27
n end
 energyBounds

e
n
e
r
g
y
B
o
u
n
d
s 2 19
p end
 energyBounds
end
 definitions
```

(continues on next page)

(continued from previous page)

```
read
 biasing

n
E
n
e
r
g
y
B
o
u
n
d
s
I
D
=1
p
E
n
e
r
g
y
B
o
u
n
d
s
I
D
=2

t
a
r
g
e
t
W
e
i
g
h
t
s 27
r1
.0 19
r0
.1  end

l
o
w
e
r
W
e
i
g
h
```

(continues on next page)

(continued from previous page)

```
end
 biasing
```

Alternatively, to use Russian roulette and splitting, the target weights and a window ratio ("windowRatio=") can be specified. The window ratio is simply the ratio of the weight window upper bound to the weight window lower bound, with the target weight being the average of the upper and lower. If target weights $\overline{w}$ and a window ratio r are supplied, then the lower and upper weight bounds are found by using

$$w_{\min} = \frac{2}{r+1}\overline{w} \tag{5.21}$$

$$w_{\max} = \frac{2r}{r+1}\overline{w} \tag{5.22}$$

If only the window ratio is supplied, both Russian roulette and splitting will be turned on with the target weights for every energy group and every region set to 1.

A target weight of 0 will prevent particles of that energy group in that region from being transported. For example, to perform a neutron-only calculation using a coupled neutron-photon library, simply set the target weight values for all of the photon groups in every region to 0. The user should be careful not to "turn off" energy groups or regions that may impact (bias incorrectly) the final tally results.

Monaco always uses the implicit capture technique—at collision sites absorption is not simulated but instead the particle weight is reduced by the ratio of the scatter probability to the total interaction probability. Particles only stop if they escape the defined geometry. This generally produces tally results with lower uncertainties in less time, but for highly scattering or very large geometries, particles with very low weights will be tracked until their weight reaches the lower limit of real numbers in double precision. This is not typically what the user wants. So, for problems that are not using any weight windows or importance map, Russian roulette and splitting are automatically turned on using the a target weight of 1 for every energy group and every region and a window ratio of 5.

Path-length stretching

Path-length stretching allows particles going a certain direction to travel farther (with reduced weight) before interacting. Seventeen different directions are available, as listed in the Table 8.2.10. One of the directions is specified by using the "direction=" keyword and one of the direction strings listed in Table 8.2.10, in quotes. The amount of stretching is specified using the "pathStretch … end" array, with values between 0 (no stretching) and 1 (lots of stretching), for each energy group and region. Items can be listed in any order. Similar to the weight window arrays, the "pathStretch" array can have a length matching (1) the product of the number of energy groups and the number of regions, (2) the number of regions, or (3) the number of energy groups. Values are repeated to fill in all of the regions and groups.

```
read
 biasing

p
a
t
h
S
t
r
e
t
c
h  46
r0
.5 46
r0
.6 46
r0
.75 end
```

(continues on next page)

(continued from previous page)

```
d
i
r
e
c
t
i
o
n
=
"
l
o
c
a
l
Z
p
"
end
 biasing
```

When stretching toward a given location (direction="location"), then the location ID number must be specified using the "locationID=" keyword. For CE calculations, energy boundary objects need to be defined using the keywords "nEnergyBoundsID=" and "pEnergyBoundsID=".

Table 5.10: Directions available for path-length stretching

Direction	Comment
`localXp`	+x direction in local coordinates
`localYp`	+y direction in local coordinates
`localZp`	+z direction in local coordinates
`localXm`	-x direction in local coordinates
`localYm`	-y direction in local coordinates
`localZm`	-z direction in local coordinates
`localYZ`	cylindrically away from x-axis (local)
`localXZ`	cylindrically away from y-axis (local)
`localXY`	cylindrically away from z-axis (local)

Direction	Comment
`globalXp`	+x direction in global coordinates
`globalYp`	+y direction in global coordinates
`globalZp`	+z direction in global coordinates
`globalXm`	-x direction in global coordinates
`globalYm`	-y direction in global coordinates
`globalZm`	-z direction in global coordinates
`outward`	spherically outward (local)
`location`	in the direction of a given location (requires a locationID)

Mesh-based importance map

The user can alternatively specify an existing Monaco mesh-based importance map—a binary file created by a previous MAVRIC calculation. The mesh importance map must be a binary file using the Monaco mesh importance map format (a *.mim file). This option is specified with the "meshImpMapFile=" keyword and the file name (and full path if necessary) in quotes.

```
read
 biasing
```

(continues on next page)

```
m
e
s
h
I
m
p
M
```

(continued from previous page)

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w
i
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R
a
t
i
o
=10
.0
end
 biasing
```

If the "meshImpMapFile=" keyword is used, most other biasing block keywords cannot be used. The keyword "windowRatio=" can be used and its default value is five.

If particles leave the importance map but are still in the defined geometry, the simulation will be stopped. If the user wants to allow importance maps that do not cover the entire problem, the keyword "allowShortImpMap" should be used in the parameters block. In that case, areas outside the mesh importance map will be treated as completely unimportant—particles will be killed outside the mesh.

Note that for the most effective use of an importance map, the source should be biased to match. This is what the MAVRIC sequence does – it produces a biased source such that sampled particles are born with a weight matching the target weight of the importance map.

Monaco input summary

Below are summaries of the Monaco blocks and their available keywords.

Table 5.11: Keywords for the cross section block

block keyword	type	length	default	required	restrictions/comments
read crossSections					
maxNumMixtures=	integer		100	no	only required if more than 100 mixtures
maxNumElements=	integer		100	no	only required if more than 100 elements in any mixture
For multi-group calculations					
ampxFileUnit=	integer			a*	unit number of AMPX working library
iceFileUnit=	integer			b*	unit number of ICE cross sections
					*required: either a) ampxFileUnit= or b) iceFileUnit=
For continuous energy calculations					
ceLibrary=	character			yes	required for CE, contained in double quotes
ceTempDefault=	real		293	no	set default temperature for CE mixtures
mixture *id*	integer			yes	non-negative integer
element	integer and real			yes	integer=z*1000+a, real=atom density
temperature=	real		293	no	temperature for this mixture (CE only)
end mixture					
For multi-group calculations					
printTotals			not present	no	prints total cross sections for each mixture
printScatters			not present	no	prints 2D cross sections for each mixture
printAngleProb			not present	no	print angles and probabilities for each mixture
printFissionChi			not present	no	print fission spectrum chi for each mixture
printExtra			not present	no	print extra 1D cross sections for each mixture
printLegendre			not present	no	print Legendre coefficients for each mixture
fullyCoupled			not present	no	treat all particles as primary particles
end crossSections					

Table 5.12: Keywords for the definitions block

block keyword	type	length	default	required	restrictions/comments
read definitions					
location *id*	integer			yes	non-negative integer, unique among positions
title=	character		none	no	contained in double quotes (title="yada yada yada")
position	real	3		yes	global coordinates (x,y,z)
end location					
Type 1: generic user-defined response (n values is histogram, n+1 values is value/function pairs)					
response id	integer			yes	non-negative integer, unique among responses
neutron/photon				yes	indicate either neutron or photon for the response type
bounds	real	n+1	none	yes*	energy bin boundaries (eV)
energyBoundsID=	integer			yes*	use a defined energyBounds objects for bounds *either bounds or energyBoundsID is required
values	real	n or n+1		yes	non-negative real numbers
end response					
Type 2: Using a cross-section from the library (usually with units of barns)					
response id	integer			yes	non-negative integer, unique among responses
neutron/photon				yes	indicate either neutron or photon for the response type
material=	integer			yes	which material
ZAID=	integer			no	which isotope (ZAID=Z*1000+A) (omit to use cross section of entire material)
MT=	integer			yes	which MT reaction number
macro			not present	no	convert units from barns to /cm using ZAID atom density
end response					
Type 3: Flux-to-Dose conversion factors					
response id	integer			yes	non-negative integer, unique among responses
specialDose=	integer			yes	special dose factor from a MG library
end response					
response id	integer			yes	non-negative integer, unique among responses
doseData=	integer			yes	generate data points from original flux-to-dose reference
noExtrapolation			not present	no	do not use SCALE energy extrapolation
end response					
Type 4: Standard multi-group response function (MG only)					
response *id*	integer			yes	non-negative integer, unique among responses
neutron/photon				yes	indicate either neutron or photon for the response type
values	real	ng		yes	non-negative real numbers
end response					
Optional keywords for any type of response					
response *id*	integer			yes	non-negative integer, unique among responses
title=	character	256	none	no	contained in double quotes (title="yada yada yada")
multiplier=	real		1.0	no	multiplier for units conversion, etc.
makeChart			not present	no	makes a *.chart file showing the input values and the mutli-group representation (for MG)
eHigh=	real			no	keep only responses values below eHigh (eV)
eLow=	real			no	keep only responses values above eLow (eV)
lessOutput			not present	no	only show first 5 and last 5 points of response
end response					
makeCharts			not present	no	makes a *.chart file for each response
multiplier=	real		1.0	no	multiplier applied to all defined responses
lessOutput			not present	no	only show first 5 and last 5 points of response
end definitions					

ng is the number of groups in the multi-group cross section library for that type of particle

Table 5.13: More keywords for the definitions block

block	keyword	type	length	default	required	restrictions/comments
read definitions						
	gridGeometry *id*				yes	non-negative integer, unique among grid geometries
	title=	character	256	none	no	contained in double quotes (title="yada yada yada")
	xplanes	real	any		no	a list of real numbers (order not important) in *x* dimension
	xLinear n min max	int real real			no	adds *n*+1 planes evenly from min to max in *x* dimension
	yplanes	real	any		no	a list of real numbers (order not important) in *y* dimension
	yLinear n min max	int real real			no	adds *n*+1 planes evenly from min to max in *y* dimension
	zplanes	real	any		no	a list of real numbers (order not important) in *z* dimension
	zLinear n min max	int real real			no	adds *n*+1 planes evenly from min to max in *z* dimension
	tolerance=	real		1.E-06	no	for removing duplicate planes from *planes or *Linear
	make3dmap			not present	no	makes a *.3dmap file showing the grid geometry
	xdivide=	integer		1	no	Once all xplanes are entered, further divide them by this
	ydivide=	integer		1	no	Once all yplanes are entered, further divide them by this
	zdivide=	integer		1	no	Once all zplanes are entered, further divide them by this
	end gridGeometry					
	make3dmaps			not present	no	makes a *.3dmap file for each of the grid geometries
	cylGeometry *id*	integer			yes	non-negative integer, unique among cylindrical geometries
	title=	character	256	none	no	contained in double quotes (title="yada yada yada")
	radii	real	any		no	list of radii
	thetas	real	any		no	list of angles (0 to 2π)
	degrees	real	any		no	list of angles (0 to 360°)
	zPlanes	real	any		no	list of zplanes (relative to position where z=0)
	radiusLinear *n min max*	int real real			no	adds *n*+1 radii evenly from min to max
	thetaLinear *n min max*	int real real			no	adds *n*+1 theta planes evenly from min to max (0 to 2π)
	degreeLinear *n min max*	int real real			no	adds *n*+1 theta planes evenly from min to max (0 to 360°)
	zLinear *n min max*	int real real			no	adds *n*+1 *z*-planes evenly from min to max
	position	real	3	(0, 0, 0)	no	position from which to start radii and zplanes
	zaxis *u v w*	real	3	<0, 0, 1>	no	set the axis of the cylindrical mesh
	xaxis *u v w*	real	3	<1, 0, 0>	no	set the reference position of the cylindrical mesh
	tolerance=	real		1.E-06	no	for removing duplicate planes from *planes or *Linear
	makeCylMap			not present	no	makes a *.3dmap file showing the cylindrical mesh
	end cylGeometry					
	makeCylMaps			not present	no	makes a *.3dmap file for each of the cylindrical geometries
end definitions						

Table 5.14: Even more keywords for the definitions block

block	keyword	type	length	default	required	restrictions/comments
read definitions						
For a histogram-type distribution of n bins						
distribution *id*		integer			yes	non-negative integer, unique among responses
	title=	character	256		no	contained in double quotes (title="yada yada yada")
	abscissa	real	n+1		yes*	bin boundaries
	truePDF	real	n		see text	binned values of the true probability distribution function
	trueCDF	real	n			binned values of the true continuous distribution function
	biasedPDF	real	n			binned values of the biased probability distribution function
	biasedCDF	real	n			binned values of the biased continuous distribution function
	weight	real	n			suggested weight for each bin
	importance	real	n			suggested importance value for each bin
	runSampleTest			not present	no	run a sampling test for this distribution (makes a *.chart file)
end distribution						
For distributions consisting of value/function pairs over n intervals						
distribution *id*		integer			yes	non-negative integer, unique among responses
	title=	character	256		no	contained in double quotes (title="yada yada yada")
	abscissa	real	n+1		yes	abscissa values
	truePDF	real	n+1		see text	point values of the true probability distribution function
	biasedPDF	real	n+1			point values of the biased probability distribution function
	weight	real	n+1			point values of the suggested weights
	importance	real	n+1			point values of the suggested importance
	runSampleTest			not present	no	run a sampling test for this distributions (makes *.chart file)
end distribution						
For histograms or value/function pairs						
distribution *id*						
	Use a defined energyBounds objects for the abscissa values					
	energyBoundsID=	integer			yes*	use boundaries from a defined energyBounds as abscissa
	For multi-group calculations					
	neutronGroups/photonGroups				yes*	use neutron/photon energy bin boundaries as abscissa values *required: abscissa, energyBoundsID, or neutron/photonGrou If not abscissa, n must match number of groups
end distribution						
For a list on n discrete values						
distribution *id*		integer			yes	non-negative integer, unique among responses
	title=	character	256		no	contained in double quotes (title="yada yada yada")
	discrete	real	n		yes	discrete values
	truePDF	real	n		see text	true probabilities
	trueCDF	real	n			true cumulative probabilities
	biasedPDF	real	n			biased probabilities
	biasedCDF	real	n			biased cumulative probabilites
	weight	real	n			suggested weight for each bin
	importance	real	n			suggested importance for each value
	runSampleTest			not present	no	run a sampling test for this distribution (makes a *.chart file)
end distribution						
end definitions						

Table 5.15: Special distribution keywords for the definitions block

block	keyword	type	length	default	required	restrictions/comments
read definitions						
For special and built-in distributions						
distribution *id*						
	special=	character	30		yes	"wattSpectrum", "cosine", "exponential", "pwrNeutronAxialProfile", "pwrGammaAxialProfile", "pwrNeutronAxialProfileReverse", "pwrGammaAxialProfileReverse", "fissionPhotons", "origensBinaryConcentrationFile", "fissionNeutrons"
	parameters	real	<=10		depends	each type of distribution could have parameters
	filename=	string		none	depends	legal file name for current system, in quotes required for special="origensBinaryConcentrationFile"
	runSampleTest			not present	no	run a sampling test for this distributions (makes *.chart file)
end distribution						
runSampleTests				not present	no	show all of the distributions and a sampling test of each
end definitions						

Table 5.16: Continuous energy keywords for the definitions block

block	keyword	type	length	default	required	restrictions/comments
read definitions						
energyBounds *id*		integer			yes	non-negative integer, unique among energyBounds objects
	title=	character	256	none	no	contained in double quotes (title="yada yada yada")
	bounds	real	any		no	a list of energy bin boundaries (in eV, order not important)
	linear *n min max*	int real real			no	adds $n+1$ boundaries (eV) evenly from min to max
	logarithmic *n min max*	int real real			no	adds $n+1$ boundaries (eV) logarithmically from min to max
	tolerance=	real		1.E-06	no	for removing duplicate boundaries from various commands
	252n			not present	no	add energy bin boundaries from 252-group neutron library
	238n			not present	no	add energy bin boundaries from 238-group neutron library
	200n			not present	no	add energy bin boundaries from 200-group neutron library
	56n			not present	no	add energy bin boundaries from 56-group neutron library
	47p			not present	no	add energy bin boundaries from 47-group photon library
	44n			not present	no	add energy bin boundaries from 44-group neutron library
	27n			not present	no	add energy bin boundaries from 27-group neutron library
	19p			not present	no	add energy bin boundaries from 19-group photon library
end energyBounds						
timeBounds *id*		integer			yes	non-negative integer, unique among timeBounds objects
	title=	character	256	none	no	contained in double quotes (title="yada yada yada")
	bounds	real	any		no	a list of time bin boundaries (in sec, order not important)
	linear *n min max*	int real real			no	adds $n+1$ boundaries (sec) evenly from min to max
	logarithmic *n min max*	int real real			no	adds $n+1$ boundaries (sec) logarithmically from min to max
	tolerance=	real		1.E-10	no	for removing duplicate boundaries from various commands
end timeBounds						
end definitions						

Table 5.17: Keywords for the sources block

block	keyword	type	length	default	required	restrictions/comments
read sources						
	Defining a source					
	src id	integer			yes	non-negative integer, unique among src objects
	title=	character	256	none	no	contained in double quotes (title="yada yada yada")
	neutron/photon				yes	indicate either neutron or photon for a source particle type
	strength=	real			yes	total source strength (particles/sec)
	biasedStrength=	real		0.0	no	strength to use for sampling this source
	(spatial dependence: at most one solid)					
	cuboid	real	6		no	parameters: x_{max} x_{min} y_{max} y_{min} z_{max} z_{min}
	xCylinder	real	3		no	parameters: r x_{max} x_{min}
	yCylinder	real	3		no	parameters: r y_{max} y_{min}
	zCylinder	real	3		no	parameters: r z_{max} z_{min}
	xShellCylinder	real	4		no	parameters: r_1 r_2 x_{max} x_{min}
	yShellCylinder	real	4		no	parameters: r_1 r_2 y_{max} y_{min}
	zShellCylinder	real	4		no	parameters: r_1 r_2 z_{max} z_{min}
	sphere	real	1		no	parameters: r
	shellSphere	real	2		no	parameters: r_1 r_2
	origin				no	change center point of geometry by adding x,y,z
	x=	real		0.0	no	
	y=	real		0.0	no	
	z=	real		0.0	no	
	cylinderAxis *u v w*	real	3	<0,0,1>	no	direction <*u*,*v*,*w*> in global coordinates of cylinder axis
	unit=	integer		-1	no	limit source to a specific unit
	region=	integer		-1	no	limit source to a specific region of a unit
	mixture=	integer		-1	no	limit source to a specific mixture
	xDistributionID=	integer		none	no	distribution for *x* component of cuboid
	xScaleDist			not present	no	scale the distribution to match *x* length
	yDistributionID=	integer		none	no	distribution for *y* component of cuboid
	yScaleDist			not present	no	scale the distribution to match *y* length
	zDistributionID=	integer		none	no	distribution for *z* comp. of cuboid or axial comp. of cylinder
	zScaleDist			not present	no	scale the distribution to match *z* length
	rDistributionID=	integer		none	no	distribution for *r* component of cylinder or sphere
	rScaleDist			not present	no	scale the distribution to match *r* length
	(energy dependence)					
	eDistributionID=	integer		none	no	distribution to use for energy sampling
	useNormConst			not present	no	set the source strength with the normalization constant of the energy distribution (do not use strength= with this)
	(directional dependence)					
	direction *u v w*	real	3	<0,0,1>	no	reference direction <*u*,*v*,*w*> in global coordinates
	dDistributionID=			none	no	distribution to use for energy sampling
	dScaleDist			not present	no	scale the distribution to match [-1,1] range
	(spatial & energy dependence together)					
	meshSourceFile=	string		not present	no	legal file name for current system, in quotes
	allowResampling			not present	no	see manual
	end src					
end sources						

Table 5.18: More keywords for the sources block

block	keyword	type	length	default	required	restrictions/comments
read sources						
	Define source(s)					
	src *id*					
	…					
	end src					
	src *id*					
	…					
	end src					
	Saving the defined source(s) as a mesh source file					
	meshSourceSaver					
	gridGeometryID=	integer			yes	matches one of the id numbers from gridGeometries
	filename=	string		"source.msm"	no	legal file name for current system, in quotes
	subCells=	integer		2	no	subcells per cell (each dimension)
	sourceTrials=	integer		1000000	no	how many source particles to sample
	reduce			not present	no	stores only the cuboid around the voxels with source
	makeTotal			not present	no	save a mesh version of the total source (if >1 source)
	For continuous energy calculations					
	nEnergyBoundsID=	integer		not present	yes*	neutron energy bins for CE-Monaco calculations
	pEnergyBoundsID=	integer		not present	yes*	photon energy bins for CE-Monaco calculations
	Advanced Options					
	sampleFromMesh			not present	no	replace the above source(s) with this mesh source
	meshBiasFile=	string		none	no	use the biasing info in a different mesh source
	end meshSourceSaver					
end sources						

Table 5.19: Keywords for the tallies block

block keyword	type	length	default	required	restrictions/comments
read tallies					
pointDetector *id*				yes	non-negative integer, unique among pointDetectors
locationID=	integer			yes	matches one of the id numbers from locations
minSampProb=	real		1.0	no	minimum sampling probability for pd calculation
end pointDetector					
regionTally *id*				yes	non-negative integer, unique among regionTallys
unit=	integer		-1	see text	limit tally to a specific unit
region=	integer		-1	see text	limit tally to a specific region of a unit
mixture=	integer		-1	see text	limit tally to a specific mixture
end regionTally					
meshTally *id*				yes	non-negative integer, unique among meshTallys
gridGeometryID=	integer			a*	matches one of the id numbers from gridGeometries
cylGeometryID=	integer			b*	matches one of the id numbers from cylGeometries
					*required: either a) gridGeometryID= or b) cylGeometryID=
unit=	integer		-1	see text	limit tally to a specific unit
region=	integer		-1	see text	limit tally to a specific region of a unit
mixture=	integer		-1	see text	limit tally to a specific mixture
noGroupFluxes			not present	no	do not write group fluxes to mesh tally file
noStatChecks			not present	no	do not perform statistical checks
saveRespDetails			not present	no	save each response (group by group) to a separate file
weightless			not present	no	without weight, this becomes an MC particle flux tally
end meshTally					
For all three tally types					
****Tally *id*					
title=	character	256	none	no	contained in double quotes (title="yada yada yada")
neutron/photon				yes	indicate either neutron or photon for a tally type
responseID=	integer		none	no	matches one of the id numbers from responses
responseIDs	integer	any	none	no	list of id numbers from responses
multiplier=	real		1.0	no	multiplier for units conversion, etc.
For continuous energy calculations					
energyBoundsID=	integer			no	default is one energy bin 0 to 100 MeV
timeBoundsID=	integer			no	default is one time bin 0 to ?? Seconds
end ****Tally					
multiplier=	real		1.0	no	multiplier for all tallies (mulitplies individual multipliers)
minSampProb=	real		1.0	no	minimum sampling probability for all point detectors
end tallies					

Table 5.20: Keywords for the parameters block

block	keyword	type	length	default	required	restrictions/comments
read parameters						
	randomSeed=	hex		0000000100000001	no	hexidecimal number
	perBatch=	integer		1000	no	positive integer
	batches=	integer		10	no	positive integer
	maxMinutes=	real		0.0	no	non-negative real number
	maximumLost=	integer		10	no	maximum number of lost particles to tolerate
	voidAllRegions			not present	no	replace all materials with voids for geometry testing
	allowShortImpMap			not present	no	particles outside importance map are killed
	noCheckAtBirth			not present	no	do not check the weight of source particles
	Particles to simulate					
	neutron			not present	no	For MG, the particles contained in the library will be
	photon			not present	no	transported unless turned off. In CE, the user should
	noNeutron			not present	no	specify which particles to transport.
	noPhoton			not present	no	
	fissionMult=	integer		2	no	production of fission neutrons (0-no, 1-one, 2-multiple)
	secondaryMult=	integer		2	no	production of gammas form neutrons (0-no, 1-one, 2-multiple)
	For continuous energy calculations					
	nMinEnergy	real		1.0E-05	no	minimum energy (eV) for neutrons
	pMinEnergy	real		1.0E+04	no	minimum energy (eV) for photons
	nMaxEnergy	real		2.0E+07	no	maximum energy (eV) for neutrons
	pMaxEnergy	real		2.0E+07	no	maximum energy (eV) for photons
	nMaxAge	real		1	no	maximum age (sec) for neutrons
	pMaxAge	real		1	no	maximum age (sec) for photons
	noPTables			not present	no	turn off the use of probability tables
	dopplerBroaden	integer		0	no	Doppler pre-broadening of cross sections (0-none, 1-1D cross sections, 2-1D and 2D cross sections)
	Legacy keywords					
	noFissions			not present	no	no production of fission neutrons (fissionMult=0)
	noSecondaries			not present	no	no production of gammas from neutrons (secondaryMult=0)
end parameters						

Table 5.21: Keywords for the biasing block

block	keyword	type	length	default	required	restrictions/comments
read biasing						
	Standard biasing techniques					
	forcedCollisions			not present	no	force particle to interact within geometry
	targetWeights	real	a*	none	no	non-negative real numbers
	lowerWeights	real	a*	none	no	non-negative real numbers
	upperWeights	real	a*	none	no	non-negative real numbers
	windowRatio=	real		none	no	real number greater than one
	pathStretch	real	a*	none	no	valid range of values: [0.0,1.0)
	direction=	string		none	no	one of 17 strings, in quotes
	locationID=	integer		none		required for direction="location"
						*a is one of {ng*nr, nr, ng}
	mapMultiplier=	real		1.0	no	multiply *Weights by this factor
	For continuous energy					
	nEnergyBoundsID=	integer		not present	no	neutron energy bins for CE-Monaco calculations
	pEnergyBoundsID=	integer		not present	no	photon energy bins for CE-Monaco calculations
	Using a Monaco mesh importance map file					
	meshImpMapFile=	string		not present	no	legal file name for current system, in quotes
	mapMultiplier=	real		1.0	no	multiply targetWeights in imp. Map
end biasing						

ng is the number of groups in the MG cross section library or in the energyBounds specified for CE
nr is the number of regions in the geometry

5.4 Monaco Output

5.4.1 Main text output file

The Monaco output file first reviews the input Monaco received. First is a review of the geometry—showing which materials are used in each region and the volume of that region, if input or calculated. Then there is a detailed list of other Monaco input: cross-section parameters, data definitions, the sources, the tallies, the Monte Carlo parameters, and the biasing parameters. For calculations using an importance map, its summary is also given. The "Mesh Importance Map Characterization" shows where the importance map may be changing too fast and may require more refinement.

For each batch of source particles simulated, the output file lists the batch time and the starting random number for the next batch, which may be useful in rerunning just a portion of a problem. Once all of the batches are completed, a list of the various tally files that have been created is given. Finally, the tallies are summarized in a section titled "Final Tally Results Summary". For each point detector, the total neutron and photon fluxes (uncollided and total) are given as well as the final response values for each response function. For each region tally, the total neutron and photon fluxes (both track-length and collision density estimates) are listed, followed by the final response values for each response function. Along with each of the final quantities are the standard deviation of the quantity, the relative uncertainty, the figure-of-merit and a summary of list of the statistical checks (passed or not).

5.4.2 Tally files

In addition to the summary of tallies contained in the Monaco text output file, many other files are created containing the group-by-group details of the final tally data. Each mesh tally produces a file "*outputName*.mt*id*.3dmap" where *outputName* is the name the user chose for his output file and "*id*" is the identification number corresponding to the tally specification. This file can be viewed using the Mesh File Viewer capability of Fulcrum. Point detector tallies and region tallies each create files "*outputName*.pd*id*.txt" or "*outputName*.rt*id*.txt" to list the group-by-group results. They also produce chart files, "*outputName*.pd*id*.chart" or "*outputName*.rt*id*.chart", which contain the total neutron flux, the total photon flux, and the total response function value calculated at the end of each batch. This data can be used to look at tally convergence and can be viewed with the Interactive Plotter capabilities of Fulcrum. Table 5.22 lists the output files, based on the name of the main output file (here called *outputName)*, that are available to the user. These files will be copied back to the directory where SCALE was executed.

5.4.3 Diagnostic files

Three of the data types defined in the definitions block can create files or add output to the main text output file to allow the user to ensure items were interpreted by Monaco as they were intended. Responses that included the "makeChart" keyword will each produce a file "*outputName*.resp*id*.chart", where "*id*" is the response identification number, which can be displayed using the Interactive Plotter. Grid geometries that include the keyword "make3dmap" will each produce a file called "*outputName*.grid*id*.3dmap", where "*id*" is the grid geometry identification number, which can be visualized using the Mesh File Viewer. Likewise, cylindrical geometries with the keyword "makeCylMap" will create a file called "*outputName*.cyl*id*.3dmap". Distributions using the "runSampleTest" keyword will produce a file "*outputName*.dist*id*.chart", where "*id*" is the response identification number. The "runSampleTest" results will also be displayed in the main text output with each distribution listed in the Monaco input review.

Table 5.22: Output files created by Monaco

Filename	Viewer	Description	
Output Summary			
	outputName.out		main text output file, contains results summary
Diagnostic Files			
	outputName.resp*id*.chart	P	response input and MULTIGROUP representation for response *id*
	outputName.grid*id*.3dmap	V	mesh version of geometry using grid geometry *id*
	outputName.cyl*id*.3dmap	V	mesh version of geometry using cylindrical geometry *id*
	outputName.dist*id*.chart	P	distribution input and sampling test for distribution *id*
Mesh Source Saver			
	filename.msm	V	mesh representation of a single source or total source
	filename.id.msm	V	mesh representation of multiple sources
	filename.sampling.msm	V	biased representation of a single source or total source
	filename.sampling.*id*.msm	V	biased representation of multiple sources
Tally Files			
	outputName.pd*id*.txt		detailed results for point detector tally *id*
	outputName.pd*id*.chart	P	batch convergence data for point detector tally *id*
	outputName.rt*id*.txt		detailed results for region tally *id*
	outputName.rt*id*.chart	P	batch convergence data for region tally *id*
	outputName.mt*id*.3dmap	V	mesh tally for meshTally *id*
	outputName.mt*id*.resp*xx*.3dmap	V	mesh tally of response by group for meshTally *id*, response *xx*
	outputName.mt*id*.flux.txt		detailed results for the group-wise flux of meshTally *id*
	outputName.mt*id*.tfluxtxt		detailed results for total flux of meshTally *id*
	outputName.mt*id*.resp*xx*.txt		detailed results for response *xx* of meshTally *id*
V – can be displayed with the Mesh File Viewer capabilities Fulcrum. P – can be displayed with the 2D plotting capabilities of Fulcrum.			

5.4.4 Mesh source saver files

If the Mesh Source Saver was used, one mesh source file will be created for each defined source. For a single source, the filename will be whatever was listed with the "filename=" keyword or "source.msm" if nothing was given. For multiple sources, the filenames will include the source identification number, such as "source.*id*.msm". If there were multiple sources and the "makeTotal" keyword was used, the total will be stored in "source.msm". Note that if these files are desired, they must be manually copied back from the SCALE temporary area.

If the keyword "meshBiasFile=" was used, then for every mesh source generated above there will also be a biased mesh source that is used in sampling. These files have the names in the form of "source.sampling.*id*.msm".

5.4.5 Statistical checks on point detector and region tallies

With each region tally and point detector tally, detailed statistical information is provided in separate files, "*outputName*.rt*id*.txt" or "*outputName*.pd*id*.txt", just after the group-by-group values for the fluxes and responses. For the total fluxes and any responses of each tally, two tables are given.

First, the values of the tally and several statistical quantities are listed as a function of batch number. With each batch, the statistical tests are listed by number with one of the following: "X" for passing, "-" for failing or a blank if the test could not be performed yet. The second table lists the details of the final statistical checks for the last batch completed. This table lists the value for each of the six tests as well as what the goal is for that test.

As an example, consider a 1 Ci point source of Watt spectrum neutrons inside an r=20 cm sphere of polyethylene. Two tallies are used to find the neutron dose rate (rem/hr) 35 cm from the center of the sphere – a region tally (region between two concentric spheres with radii of 34 and 36 cm) and a point detector 35 cm away from the center of the sphere. Twenty batches of 1000 particles each were used in this example.

The first depiction of the region tally dose rate response is shown in Listing 5.1. Since four of the tests involve curve fits to the table values over the last half of the simulation, the table is split showing each half of the simulation separately. The second depiction of the region tally, showing all of the details for the last batch, is shown in Listing 5.2. These two tables show that this tally passed all the statistical tests for the entire second half of the simulation. This information, combined with the fact that this is a simple tally for a well-posed problem, indicates that this tally is well converged.

Listing 5.1: Tally values for a well-converged tally.

```
T
a
l
l
y
V
a
l
u
e
s
a
s
t
h
e
S
i
m
u
l
```

(continues on next page)

```
a
t
i
o
n
P
r
```

(continued from previous page)

```
a
v
e
r
a
g
e
s
t
a
n
d
a
r
d
r
e
l
a
t
r
e
l
F
O
M
s
t
a
t
s
c
h
e
c
k

b
a
t
c
h
v
a
l
u
e
d
e
v
i
a
t
i
o
n
u
n
c
e
r
t
```

(continues on next page)

(continued from previous page)

(continues on next page)

(continued from previous page)

```
            1  2
.06269
E
+01  2
.45012
E
+00  0
.11878  1
.45
E
-02  9
.96
E
+02
-
X
            2  1
.87353
E
+01  1
.65492
E
+00  0
.08833  8
.16
E
-03  8
.76
E
+02
-
X
            3  1
.82317
E
+01  1
.33026
E
+00  0
.07296  5
.63
E
-03  8
.45
E
+02
-
X
            4  1
.80905
E
+01  1
.15401
E
+00  0
.06379  4
.27
E
-03  8
.28
E
+02
-
X
```

(continues on next page)

(continued from previous page)

```
            5  1
.82780
E
+01  1
.03792
E
+00  0
.05679  3
.40
E
-03  8
.36
E
+02
-
X
            6  1
.75679
E
+01  9
.28759
E
-01  0
.05287  2
.97
E
-03  8
.00
E
+02
-
X
            7  1
.71843
E
+01  8
.46577
E
-01  0
.04926  2
.60
E
-03  7
.89
E
+02
X
X
            8  1
.74775
E
+01  7
.99275
E
-01  0
.04573  2
.23
```

(continues on next page)

```
E
-03  8
.03
E
+02
X
X
```

(continued from previous page)

```
           9  1
.73520
E
+01  7
.52502
E
-01  0
.04337  2
.00
E
-03  7
.94
E
+02
X
X
          10  1
.76020
E
+01  7
.17178
E
-01  0
.04074  1
.76
E
-03  8
.11
E
+02
X
X
X
X
X
X

          11  1
.74628
E
+01  6
.80834
E
-01  0
.03899  1
.62
E
-03  8
.03
E
+02
X
X
X
X
X
X
```

(continues on next page)

(continued from previous page)

```
          12  1
.75161
E
+01  6
.52464
E
-01  0
.03725  1
.48
E
-03  8
.08
E
+02
X
X
X
X
X
X
          13  1
.72561
E
+01  6
.21777
E
-01  0
.03603  1
.39
E
-03  7
.96
E
+02
X
X
X
X
X
X
          14  1
.73196
E
+01  6
.00329
E
-01  0
.03466  1
.29
E
-03  8
.00
E
+02
X
X
X
X
X
X
```

(continues on next page)

(continued from previous page)

```
          15  1
.72025
E
+01  5
.77747
E
-01  0
.03359  1
.21
E
-03  7
.97
E
+02
X
X
X
X
X
X
          16  1
.72019
E
+01  5
.58956
E
-01  0
.03249  1
.14
E
-03  7
.98
E
+02
X
X
X
X
X
X
          17  1
.72998
E
+01  5
.43721
E
-01  0
.03143  1
.06
E
-03  8
.02
E
+02
X
X
X
X
X
X
```

(continues on next page)

(continued from previous page)

```
          18  1
.73534
E
+01  5
.29351
E
-01  0
.03050  9
.99
E
-04  8
.06
E
+02
X
X
X
X
X
X
          19  1
.72752
E
+01  5
.14264
E
-01  0
.02977  9
.51
E
-04  8
.01
E
+02
X
X
X
X
X
X
          20  1
.74155
E
+01  5
.03061
E
-01  0
.02889  8
.95
E
-04  8
.08
E
+02
X
X
X
X
X
X
```

(continues on next page)

(continued from previous page)

(continues on next page)

(continued from previous page)

Listing 5.2: Final check for a well-converged tally.

```
F
i
n
a
l
S
t
a
t
i
s
t
i
c
a
l
C
h
e
c
k
(
f
i
t
s
a
r
e
o
v
e
r
t
h
e
l
a
s
t
h
a
l
f
o
f
t
h
e
s
i
m
u
l
a
t
i
o
n
)
```

(continues on next page)

(continued from previous page)

```
q
u
a
n
t
i
t
y
c
h
e
c
k
g
o
a
l
a
c
t
u
a
l
p
a
s
s

-
-
-
```

(continued from previous page)

```
      1
m
e
a
n
r
e
l
s
l
o
p
e
o
f
l
i
n
e
a
r
f
i
t
=  0
.00
-0
.0118
y
e
s
      2
s
t
a
n
d
a
r
d
d
e
v
i
a
t
i
o
n
e
x
p
o
n
e
n
t
o
f
p
o
w
e
r
```

(continues on next page)

(continued from previous page)

```
      3
r
e
l
a
t
i
v
e
u
n
c
e
r
t
a
i
n
t
y
f
i
n
a
l
v
a
l
u
e
<  0
.05    0
.0289
y
e
s
      4
r
e
l
a
t
i
v
e
V
O
V
e
x
p
o
n
e
n
t
o
f
p
o
w
e
r
f
.
```

(continues on next page)

(continued from previous page)

```
      5
r
e
l
a
t
i
v
e
V
O
V
f
i
n
a
l
v
a
l
u
e
<  0
.10    0
.0009
y
e
s
      6
f
i
g
u
r
e
-
o
f
-
m
e
r
i
t
(
F
O
M
)
r
e
l
s
l
o
p
e
o
f
l
i
n
e
a
```

(continues on next page)

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Since the point detector is close compared to the size of the sphere, it should converge slower than the region tally. Contributions coming from different parts of the sphere have large differences in attenuation which will cause large fluctuations in the weights arriving at the point detector. The two statistical tables are shown in Listing 5.3 and Listing 5.4. This tally is not yet converged enough to pass most of the statistical tests. With thirty times the simulation time, this point detector tally will pass all six tests.

Fig. 5.14 shows the behavior of both the region tally (well-converged) and the point detector tally (not-yet-converged) for this example problem as a function of the simulation run time (shown as the twenty batches of particles). The batch values are shown as blue points and the fits for the last half of the simulation are shown as solid black lines. The average value for a tally should be constant, so test 1 looks at the slope of a linear fit over the tally average over the last half of the simulation. The uncertainty of the tally should decrease with the square root of the total number of particles ($\frac{1}{\sqrt{N}}$), so test 3 computes the slope of an exponential fit which should be close to -0.5 (green dotted line). The variance-of-the-variance (VOV) should decrease with $\frac{1}{N}$, so test 4 computes the slope of an exponential fit which should be close to -1.0. The tally figure-of-merit (FOM) should be constant. Test 6 computes the slope of the FOM values which should be zero.

Listing 5.3: Tally values for a not-yet-converged tally.

```
T
a
l
l
y
V
a
l
u
e
s
a
s
t
h
e
S
i
m
u
l
a
t
i
o
n
P
r
o
g
r
e
s
s
e
d
```

(continues on next page)

(continued from previous page)

```
averagestandardrelatrelFOMstatschecks

batchvaluedeviationun
certainty
```

(continues on next page)

(continued from previous page)

(continues on next page)

(continued from previous page)

```
            1  1
.45258
E
+01  3
.00915
E
+00  0
.20716  1
.60
E
-01  3
.27
E
+02
-
-
            2  1
.83822
E
+01  4
.47657
E
+00  0
.24353  5
.27
E
-01  1
.15
E
+02
-
-
            3  1
.84192
E
+01  3
.44084
E
+00  0
.18681  3
.20
E
-01  1
.29
E
+02
-
-
            4  1
.87897
E
+01  2
.80685
E
+00  0
.14938  2
.33
E
-01  1
.51
E
+02
-
-
```

(continues on next page)

(continued from previous page)

```
            5  1
.78133
E
+01  2
.31117
E
+00  0
.12974  2
.09
E
-01  1
.60
E
+02
-
-
            6  1
.75190
E
+01  2
.02252
E
+00  0
.11545  1
.74
E
-01  1
.68
E
+02
-
-
            7  1
.79523
E
+01  2
.18108
E
+00  0
.12149  1
.78
E
-01  1
.30
E
+02
-
-
            8  1
.75624
E
+01  1
.95272
E
+00  0
.11119  1
.63
E
-01  1
.36
E
+02
-
-
```

(continues on next page)

(continued from previous page)

```
            9  1
.67648
E
+01  1
.75017
E
+00  0
.10440  1
.58
E
-01  1
.37
E
+02
-
-
           10  1
.70234
E
+01  1
.66732
E
+00  0
.09794  1
.30
E
-01  1
.40
E
+02
X
X
-
-
-
-

           11  1
.70104
E
+01  1
.55192
E
+00  0
.09123  1
.18
E
-01  1
.47
E
+02
-
-
-
X
-
-
```

(continues on next page)

(continued from previous page)

```
          12  1
.71598
E
+01  1
.48432
E
+00  0
.08650  1
.03
E
-01  1
.50
E
+02
X
-
-
X
-
-
          13  1
.74796
E
+01  1
.42808
E
+00  0
.08170  8
.85
E
-02  1
.55
E
+02
X
-
-
-
X
-
          14  1
.68710
E
+01  1
.33186
E
+00  0
.07894  8
.70
E
-02  1
.54
E
+02
X
-
-
-
X
-
```

(continues on next page)

(continued from previous page)

```
          15  1
.65807
E
+01  1
.25707
E
+00  0
.07582  8
.34
E
-02  1
.56
E
+02
X
-
-
-
X
-
          16  1
.65731
E
+01  1
.20836
E
+00  0
.07291  7
.61
E
-02  1
.59
E
+02
X
-
-
X
X
-
          17  1
.62390
E
+01  1
.14550
E
+00  0
.07054  7
.40
E
-02  1
.59
E
+02
X
-
-
```

(continues on next page)

```
X
X
-
```

(continued from previous page)

```
          18  1
.70002
E
+01  1
.17106
E
+00  0
.06889  5
.75
E
-02  1
.58
E
+02
X
-
-
X
X
-
          19  1
.70863
E
+01  1
.14126
E
+00  0
.06679  5
.20
E
-02  1
.59
E
+02
X
-
-
-
X
-
          20  1
.68215
E
+01  1
.09329
E
+00  0
.06499  5
.04
E
-02  1
.60
E
+02
X
-
-
```

(continues on next page)

```
-
X
-
```

(continued from previous page)

(continues on next page)

(continued from previous page)

Listing 5.4: Final check for a not-yet-converged tally.

```
F
i
n
a
l
S
t
a
t
i
s
t
i
c
a
l
C
h
e
c
k
(
f
i
t
s
a
r
e
o
v
e
r
t
h
e
l
a
s
t
h
a
l
f
o
f
t
h
e
s
i
m
u
l
a
t
i
o
n
)
```

(continues on next page)

(continued from previous page)

```
q
u
a
n
t
i
t
y
c
h
e
c
k
g
o
a
l
a
c
t
u
a
l
p
a
s
s

-
-
-
```

(continued from previous page)

```
      1
m
e
a
n
r
e
l
s
l
o
p
e
o
f
l
i
n
e
a
r
f
i
t
=  0
.00
-0
.0468
y
e
s
      2
s
t
a
n
d
a
r
d
d
e
v
i
a
t
i
o
n
e
x
p
o
n
e
n
t
o
f
p
o
w
e
r
```

(continues on next page)

(continued from previous page)

```
      3
r
e
l
a
t
i
v
e
u
n
c
e
r
t
a
i
n
t
y
f
i
n
a
l
v
a
l
u
e
<  0
.05    0
.0650
n
o
      4
r
e
l
a
t
i
v
e
V
O
V
e
x
p
o
n
e
n
t
o
f
```

(continues on next page)

```
p
o
w
e
r
f
i
```

(continued from previous page)

```
      5
r
e
l
a
t
i
v
e
V
O
V
f
i
n
a
l
v
a
l
u
e
<  0
.10    0
.0504
y
e
s
      6
f
i
g
u
r
e
-
o
f
-
m
e
r
i
t
(
F
O
M
)
r
e
l
s
l
o
p
e
o
f
l
i
n
e
a
```

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Fig. 5.14: Behavior of two tallies as a function of number of particle batches.

Note that the slope of the VOV is found by fitting an exponential curve through the calculated VOV values and is very sensitive to outliers. Users need to apply their own judgment to whether or not the VOV test implemented in Monaco is too strict (failing when the tally seems converged).

Mesh tallies produce similar tables - detailed statistical information is provided in separate files, "*outputName*.mt*id*.flux.txt" and "*outputName*.mt*id*.resp*xx*.txt", for the total flux and responses. First, the statistical values related to the mean relative variance are listed as a function of batch number. With each batch, the statistical tests are listed by number with one of the following: "X" for passing, "-" for failing or a blank if the test could not be performed yet. The second table lists the details of the final statistical checks for the last batch completed. This table lists the value for each of the four tests as well as what the goal is for that test.

5.5 Example Problems

5.5.1 Neutron transmission through an iron sphere

In the early 1990s, several experiments were performed in order to benchmark ENDF/B-VI cross-section data for iron [SWA93] This example problem will use Monaco to simulate one of these experiments: transmission of ^{252}Cf neutrons through a sphere of iron. The Monaco calculations will be compared to two sets of measurements, one by the Czechoslovakian National Research Institute (NRI) and the other by the Skoda Company.

The Monaco model for this sample problem (samplesinputmonaco.ironSphere.inp) will be quite simple—just a point source and a spherical shell of iron. Three different tallies are used which should all give the same result: a region tally (for a thin spherical shell at radius=100cm); a point detector tally at (x,y,z)=(100,0,0); and a coarse mesh tally, with one cell enclosing the point (x,y,z)=(100,0,0).

Input

First, the cross sections need to be computed. Here, csas-mg is used and the "activities" material is included to make sure the flux-to-dose conversion factors are added to the working library.

```
=csas-mg

M
a
t
e
r
i
a
l
s
f
o
r
L
e
a
k
a
g
e
s
p
e
c
t
r
u
m
o
f
C
f
-252
t
h
r
```

(continues on next page)

```
o
u
g
h
a
n
i
```

(continued from previous page)

```
v7
-27
n19
g
read
 composition

w
t
p
t
S
p
h
e
r
e 3 8
.0 7   26054 5
.767   26056 91
.618  26057 2
.187
                        26058 0
.298    6000 0
.07    15000 0
.03
                        16000 0
.03
        1
.0 293
.0 end

a
c
t
i
v
i
t
i
e
s 99 1
.0 293
.0 end
end
 composition
end
```

The Monaco input file starts with module name ("monaco") and a title.

```
=monaco

L
e
a
k
a
g
e
s
p
e
c
t
```

(continues on next page)

(continued from previous page)

The mixing table information can be found in the output of the above csas-mg run.

```
read
 crossSections

a
m
p
x
F
i
l
e
U
n
i
t
=4

m
i
x
t
u
r
e 3

e
l
e
m
e
n
t     26054 5.150920E-03

e
l
e
m
e
n
t     26056 7.891181E-02

e
l
e
m
e
n
t     26057 1.850588E-03

e
l
e
m
e
n
t     26058 2.478141E-04
```

(continues on next page)

(continued from previous page)

```
e
l
e
m
e
n
t      6000 2.807736E-04

e
l
e
m
e
n
t     15031 4.666202E-05

e
l
e
m
e
n
t     16032 4.283109E-05

e
l
e
m
e
n
t     16033 3.380690E-07

e
l
e
m
e
n
t     16034 1.897694E-06

e
l
e
m
e
n
t     16036 9.015172E-09
    end
 mixture
end
 crossSections
```

The SGGP geometry consists of several nested spheres. The regions (in order) are a void for the ^{252}Cf source, the iron shield, a void out to the detector, a thin shell about 100 cm, and then a void to the problem boundary. The only volume that needs to be supplied is the fourth region, since that is where the flux tally will be.

```
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

s
p
h
e
r
e   10   1
.25

s
p
h
e
r
e   11  25
.0

s
p
h
e
r
e   12  99
.5

s
p
h
e
r
e   13  100
.5

s
p
h
e
r
e   99  200
.0

m
e
d
i
a  0 1   10
v
e
l
=8
.181230869
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  3 1   11
-10
v
o
l
=65441
.66572

m
e
d
i
a  0 1   12
-11
v
o
l
=4060822
.14

m
e
d
i
a  0 1   13
-12
v
o
l
=125664
.7533

m
e
d
i
a  0 1   99
-13
v
o
l
=29258384
.9

b
o
u
n
d
a
r
y 99
```

(continues on next page)

(continued from previous page)

```
end
 geometry
```

For the different tallies, responses, locations, and grid geometry objects need to be defined. For the source, one distribution needs to be defined.

```
read
 definitions

r
e
s
p
o
n
s
e 1

t
i
t
l
e
="ANSI standard (1977) neutron flux-to-dose-rate factors  (rem/h)/(neutrons/cm2/s)"

s
p
e
c
i
a
l
D
o
s
e
=9029
    end
 response

l
o
c
a
t
i
o
n 1

t
i
t
l
e
="true detector location"

p
o
s
i
t
i
o
n 100
```

(continues on next page)

(continued from previous page)

```
    end
 location

g
r
i
d
G
e
o
m
e
t
r
y 1

t
i
t
l
e
="simple grid"

x
p
l
a
n
e
s
-25
-15
-5 5 15 25 35 55 75 95 105 end

y
L
i
n
e
a
r 5
-25 25

z
L
i
n
e
a
r 5
-25 25
    end
 gridGeometry

d
i
s
t
r
i
b
u
t
i
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="Cf-252 neutrons, Watt spectrum a=1.025 MeV and  b=2.926/MeV"

s
p
e
c
i
a
l
="wattSpectrum"

p
a
r
a
m
e
t
e
r
s 1
.025 2
.926 end
    end
 distribution
end
 definitions
```

The ^{252}Cf source can be modeled using the Watt spectrum with a=1.025 MeV and b=2.926/MeV, which was used for distribution 1. The strength is set so that the total flux at the detector (at r=100 cm) without the shield would be 1 n/cm^2/s. So, strength = 4(100)^2 = 125664 n/s.

```
read
 sources

s
r
c 1

t
i
t
l
e
="Cf-252 neutrons, Watt Spectra using a=1.025 MeV and b=2.926/MeV"

n
e
u
t
r
```

(continues on next page)

```
o
n
s
t
r
e
n
```

(continued from previous page)

```
s
p
h
e
r
e 0
.1

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources
```

Three tallies will be defined: a region tally over the fourth region of unit 1 (since this is a symmetric problem); a mesh tally using a coarse mesh over the entire problem; and a point detector tally at the true detector location.

```
read
 tallies

r
e
g
i
o
n
T
a
l
l
y 4

t
i
t
l
e
="example region tally"

n
e
u
t
r
o
n
```

(continues on next page)

(continued from previous page)

```
u
n
i
t
=1
r
e
g
i
o
n
=4

r
e
s
p
o
n
s
e
I
D
=1
    end
 regionTally




m
e
s
h
T
a
l
l
y 1

t
i
t
l
e
="example mesh tally"

n
e
u
t
r
o
n

g
r
i
d
g
e
o
m
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e
I
D
=1
    end
 meshTally

p
o
i
n
t
D
e
t
e
c
t
o
r 2

t
i
t
l
e
="example point detector"

n
e
u
t
r
o
n

l
o
c
a
t
i
o
n
I
D
=1

r
e
s
p
o
n
s
e
```

(continues on next page)

(continued from previous page)

```
    end
 pointDetector
end
 tallies
```

Monte Carlo parameters include the starting random number seed, the number of particles per batch, and the number of batches to simulate. Since we are only interested in simulating neutrons, use the keywords "neutrons" and "noPhotons" to transport neutrons and not photons. To prevent the production of fission neutrons and secondary gamma rays from neutron interactions, the keywords "fissionMult=0" and "secondaryMult=0" are used. In order to prevent a long run time, a maximum allowable run time using the "maxMinutes=" keyword could also be used.

```
read
 parameters

r
a
n
d
o
m
S
e
e
d
=8655745262010033

p
e
r
B
a
t
c
h
=262000
b
a
t
c
h
e
s
=10

n
e
u
t
r
o
n
s
n
o
P
h
o
t
o
n
s
```

(continues on next page)

(continued from previous page)

```
f
i
s
s
i
o
n
M
u
l
t
=0
s
e
c
o
n
d
a
r
y
M
u
l
t
=0
end
 parameters
```

Without any biasing parameters, Monaco will set the target weights of every energy group in every region to 1 and the values for weight lower bounds (Russian roulette) will be 1/3. Since "noPhotons" was listed in the parameters block, photons should not be generated. So, no biasing block is required.

If desired, a biasing block could be added to change the size of the weight windows (default is 5, giving lower weights of 1/3 and upper weights of 5/3). By using the default target weights of 1.0 and defining the windowRatio as 199, the lower weights are all set to 0.01 and the upper weights for splitting are 1.99.

```
read
 biasing

w
i
n
d
o
w
R
a
t
i
o
=199
.0
end
 biasing
```

or the target weights and lower weights could be listed for every group, every region or for every group/region. For all regions having the same targets and lower bounds, the following could be used:

```
read
 biasing

t
a
r
g
e
t
W
e
i
g
h
t
s  27
r1
.00 19
r0
.0 end

l
o
w
e
r
W
e
i
g
h
t
s   27
r0
.01 19
r0
.0 end
end
 biasing
```

If this last case were used, the "noPhotons" keyword would not be required since the target weights for all photon groups were explicitly set to 0.

Finally, the Monaco input file is ended with

```
end
 data
end
```

The complete input file `monaco.ironSphere.inp` is located in the SCALE `samples\input` directory.

Output

When Monaco finishes, there are several output files produced. First, the main output file lists summaries for each of the region tallies and point detector tallies. With each mesh tally, a *.3dmap file is produced which can be viewed with the Mesh File Viewer capabilities of Fulcrum. Region tallies and point detectors produce text files listing group-by-group results for fluxes and any optional responses. Both of these tallies also produce *.chart files which contain information about how the simulation progresses with each batch. These can be viewed with the Interactive Plotter capabilities of Fulcrum.

From the main output file, the final tally results summary is shown below:

```
F
i
n
a
l
T
a
l
l
y
R
e
s
u
l
t
s
S
u
m
m
a
r
y

=
=
=
```

(continued from previous page)

```
Neutronpoint Detector 2
.example point detector

average standard
```

(continues on next page)

(continued from previous page)

```
t
a
l
l
y
/
q
u
a
n
t
i
t
y
v
a
l
u
e
d
e
v
i
a
t
i
o
n
u
n
c
e
r
t
(
/
m
i
n
)   1 2 3 4 5 6

-
-
-
```

(continued from previous page)

```
u
n
c
o
l
l
i
d
e
d
f
l
u
x     5
.28059
E
-03  3
.15856
E
-06  0
.00060

t
o
t
a
l
f
l
u
x          9
.76163
E
-01  1
.06422
E
-03  0
.00109  8
.39
E
+04
X
X
X
X
X
X

r
e
s
p
o
n
s
e 1          7
.55800
E
-05  8
.05873
E
-08  0
.00114  7
```

(continues on next page)

(continued from previous page)

(continues on next page)

(continued from previous page)

```
NeutronRegionTally 4.exampleregionta
lly

averagestandardrela
tr
OMs
```

(continues on next page)

(continued from previous page)

```
t
a
l
l
y
/
q
u
a
n
t
i
t
y
v
a
l
u
e
d
e
v
i
a
t
i
o
n
u
n
c
e
r
t
(
/
m
i
n
)   1 2 3 4 5 6

-
-
-
```

(continued from previous page)

```
t
o
t
a
l
f
l
u
x
(
t
l
)     9
.75719
E
-01  5
.54774
E
-05  0
.00006  3
.09
E
+07
X
X
X
X
X
X

t
o
t
a
l
f
l
u
x
(
c
d
)     0.00000E+00

r
e
s
p
o
n
s
e 1          7
.55800
E
-05  8
.63873
E
-08  0
.00114  7
.04
E
+04
X
```

(continues on next page)

(continued from previous page)

(continues on next page)

(continued from previous page)

The fluxes reported are the total fluxes. Note the close agreement between the point detector flux and the region tally track-length estimate. The region tally did not produce a collision-density estimate of flux since the region was a void. Also notice that the neutron dose (response 1) from both tallies match well. The tally details that are saved in the *.pd*.txt or *.rt*.txt files are shown in Table 5.23. Group values for the mesh tally were obtained through the Mesh File Viewer.

For the mesh tally, the total neutron flux and neutron dose can be visualized using the Mesh File Viewer, as shown in Fig. 5.15 and Fig. 5.16. Using the mouse in the viewer, the flux and the dose rate for the cell that contains the detector location (100,0,0) are found to be 1.004 $\pm$ 2.3% n/cm^2/s and 7.82×10^{-5} $\pm$ 2.4% rem/hr, respectively, matching the other tallies well, given the higher uncertainties for the mesh tally.

A comparison of the results of all three Monaco tallies to the two experimental measurements is shown in Fig. 5.17 through Fig. 5.21 for different cross section libraries. Note that the point detector results and the region tally results are the same for most of the energy range shown. The line representing the mesh tally result becomes broken in some plots because no neutrons of certain energy groups crossed this particular mesh cell. These four plots are each for 10 minutes of computation using a 2 GHz Linux processor.

Using the library with finer groups, the Monaco results show more of the structure seen in the experiments over the energy range from 0.01 MeV to 1.0 MeV, as shown in Fig. 5.18 and Fig. 5.19.

Table 5.23: Group-by-group details of the three flux tallies (ENDF/B-VII.0 27n19g)

Energy	Mesh Tally		**Point detector**		Region Tally	
(MeV)	**value**	**rel-unc**	**value**	**rel-unc**	**value**	**rel-unc**
2.000E+07	9.59E-04	0.6325	1.30E-03	0.0344	1.35E-03	0.0168
6.376E+06	1.26E-02	0.1472	8.19E-03	0.0117	8.40E-03	0.0067
3.012E+06	2.03E-02	0.1413	2.21E-02	0.0060	2.21E-02	0.0041
1.827E+06	2.88E-02	0.0919	2.41E-02	0.0047	2.42E-02	0.0039
1.423E+06	8.94E-02	0.0770	9.05E-02	0.0026	9.06E-02	0.0020
9.072E+05	3.40E-01	0.0466	3.26E-01	0.0018	3.25E-01	0.0009
4.076E+05	4.19E-01	0.0320	4.15E-01	0.0017	4.15E-01	0.0007
1.111E+05	7.25E-02	0.0790	6.65E-02	0.0046	6.64E-02	0.0023
1.503E+04	1.27E-02	0.1751	1.21E-02	0.0118	1.21E-02	0.0055
3.035E+03	4.05E-03	0.3065	4.80E-03	0.0179	4.75E-03	0.0083
5.830E+02	1.51E-03	0.4935	2.58E-03	0.0237	2.59E-03	0.0109
1.013E+02	6.10E-04	0.6476	1.26E-03	0.0320	1.20E-03	0.0151
2.902E+01	4.75E-04	0.6724	7.23E-04	0.0367	7.16E-04	0.0182
1.068E+01	2.82E-04	0.9487	5.19E-04	0.0402	5.03E-04	0.0210
3.059E+00			1.60E-04	0.0597	1.40E-04	0.0403
1.855E+00			7.91E-05	0.0824	8.31E-05	0.0534
1.300E+00			3.15E-05	0.1059	2.96E-05	0.0901
1.125E+00			2.24E-05	0.1108	1.97E-05	0.1086
1.000E+00			3.21E-05	0.1299	2.45E-05	0.0979
8.000E-01			4.20E-05	0.1127	3.63E-05	0.0816
4.140E-01			1.02E-05	0.1720	1.03E-05	0.1583
3.250E-01			1.13E-05	0.2433	7.62E-06	0.1701
2.250E-01			8.26E-06	0.2554	7.42E-06	0.1746
1.000E-01			1.00E-06	0.4480	6.73E-07	0.6451
5.000E-02			6.61E-08	0.4590		
3.000E-02			6.59E-10	0.4491		
1.000E-02			6.90E-13	0.3458		
1.000E-05						

Fig. 5.15: Total neutron flux in n/cm2/s.

Fig. 5.16: Neutron dose rate in rem/hr.

Fig. 5.17: Comparison of Monaco results using the ENDF/B-VII.0 27n/19g library and the measured values.

Fig. 5.18: Comparison of Monaco results using the new ENDF/B-VII.0 200n/47g library and the measured values.

Fig. 5.19: Comparison of Monaco results using the ENDF/B-VII 238n library and the measured values.

Fig. 5.20: Comparison of Monaco results using the ENDF/B-VII 252n library and the measured values.

Fig. 5.21: Comparison of Monaco results using the ENDF/B-VII CE n/p library (binned using the 200n group structure) and the measured values.

5.5.2 Neutrons through a heavy water sphere

Similar to the first example problem, ^{252}Cf neutrons were measured outside of a sphere filled with heavy water [JTN+97] Two measurements were made: one without the iron/polyethylene shield and one with the shield. These two measurements were subtracted to account for scatter from the floor (which is about a 5% effect for energies above 10 keV). A great amount of detail is given for the materials and geometry of the source holder, insertion tube, and detectors in Ref. 6. For this sample problem, just the basics will be modeled in two inputs: `monaco.d2oSphereA.inp` and `monaco.d2oSphereB.inp`, both located in the SCALE `samples\input` directory.

Fig. 5.22: Experimental setup.

Input

First, the cross sections for four materials need to be computed. Here, csas-mg is used:

```
=csas-mg

L
e
a
k
a
g
e
s
p
e
c
t
r
u
m
o
f
C
f
-252
t
h
r
o
u
g
```

(continues on next page)

(continued from previous page)

```
v7
-27
n19
g
read
 composition

d2
o          1 0
.99286 293
.0 end

h2
o          1 0
.00714 293
.0 end

p
o
l
y
e
t
h
y
l
e
n
e 2 0
.882   293
.0 end

b
o
r
o
n        2 0
.118   293
.0 end

i
r
o
n         3 1
.0     293
.0 end

o
r
c
o
n
c
r
e
t
e   4 1
.0     293
.0 end
```

(continues on next page)

(continued from previous page)

```
end
 composition
end
```

The Monaco input file starts with module name ("monaco") and a title.

```
=monaco

L
e
a
k
a
g
e
s
p
e
c
t
r
u
m
o
f
C
f
-252
t
h
r
o
u
g
h
a
h
e
a
v
y
w
a
t
e
r
s
p
h
e
r
e
,
s
h
i
e
l
d
i
n
p
l
a
```

(continues on next page)

(continued from previous page)

The mixing table information can be found in the output of the above csas-mg run. The newer ENDF/B-VII libraries contain isotopic data for iron, instead of just the elemental data in the older ENDF/B-V libraries.

```
read
 crossSections

a
m
p
x
F
i
l
e
U
n
i
t
=4


m
i
x
t
u
r
e 1

e
l
e
m
e
n
t    1002     6.60172E-02

e
l
e
m
e
n
t    8016     3.32469E-02

e
l
e
m
e
n
t    1001     4.76617E-04
    end
 mixture


m
i
x
t
u
r
e 2

e
l
e
m
e
n
t    8016     3.55123E-02

m
i
x
t
u
r
e 4

e
l
e
m
e
n
t   26054     1.12815E-05

e
l
e
m
e
n
t   26056     1.77096E-04

e
l
e
m
e
n
t   26057     4.08991E-06

e
l
e
m
e
n
t   26058     5.44292E-07

e
l
e
m
e
n
t    1001     8.50077E-03

e
l
e
m
e
n
t    6000     2.01991E-02

e
l
e
m
e
n
t    8016     3.55123E-02
```

The SGGP geometry consists of two nested spheres for the source and heavy water sphere. Four cylindrical shields made of either borated polyethylene or iron are placed between the sphere and the detector position (75,0,0). The experiment sat 2 m above the floor of an experimental hall that measured 10 × 13 × 25 m. Here, the origin corresponds to the source at the center of the heavy water sphere.

```
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

s
p
h
e
r
e    10   0
.5

s
p
h
e
r
e    11  15
.0

s
p
h
e
r
e    21   2
.0
o
r
i
g
i
n
x
=75
.0

x
c
y
l
i
n
d
e
r 31  15
 26
.0 31
.0
```

(continues on next page)

(continued from previous page)

```
x
c
y
l
i
n
d
e
r 32  11
.25 31
.0 39
.0

x
c
y
l
i
n
d
e
r 33   9
.00 39
.0 47
.0

x
c
y
l
i
n
d
e
r 34   7
.25 47
.0 55
.0

c
u
b
o
i
d    41  650
.0
-650  500
-500   2300
-200

c
u
b
o
i
d    42  750
.0
-750  600
-600   2400
-500
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  0 1   10

m
e
d
i
a  1 1   11
-10

m
e
d
i
a  0 1   21
v
o
l
=33
.510322

m
e
d
i
a  3 1   31

m
e
d
i
a  2 1   32

m
e
d
i
a  2 1   33

m
e
d
i
a  2 1   34

m
e
d
i
a  0 1   41
-11
-21
-31
-32
-33
-34
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  4 1   42
-41

b
o
u
n
d
a
r
y 42
end
 geometry
```

A second input file (`samples\input\monaco.d2oSphereA.inp`) was created for the geometry without the four xcylinder shields in place.

For this example, a point detector will be used to calculate the flux at the detector location and the source will require a Watt distribution.

```
read
 definitions

l
o
c
a
t
i
o
n 1

t
i
t
l
e
="true detector location"

p
o
s
i
t
i
o
n 75
.0 0
.0 0
.0
    end
 location
```

(continues on next page)

(continued from previous page)

```
d
i
s
t
r
i
b
u
t
i
o
n 1

t
i
t
l
e
="Cf-252 neutrons, Watt spectrum a=1.025 MeV and  b=2.926/MeV"

s
p
e
c
i
a
l
="wattSpectrum"

p
a
r
a
m
e
t
e
r
s 1
.025 2
.926 end
    end
 distribution
end
 definitions
```

The strength is set so that the total flux at the detector (at r=75 cm) without any shield would be 1 n/cm^2/s. So, strength = 4(75)^2 = 70686 n/s.

```
read
 sources

s
r
c 1
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="Cf-252 neutrons, Watt fission spectrum, using a=1.025 and b=2.926"

n
e
u
t
r
o
n
s
s
t
r
e
n
g
t
h
=70685
.834704

s
p
h
e
r
e 0
.1

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources
```

Two tallies will be defined: a region tally over the third region of unit 1 and a point detector tally at the true detector

location.

```
read
 tallies

r
e
g
i
o
n
T
a
l
l
y 3

t
i
t
l
e
="example region tally"

n
e
u
t
r
o
n

u
n
i
t
=1
r
e
g
i
o
n
=3
    end
 regionTally




p
o
i
n
t
D
e
t
e
c
t
r 2
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="example point detector"

n
e
u
t
r
o
n

l
o
c
a
t
i
o
n
I
D
=1
    end
 pointDetector
end
 tallies
```

Monte Carlo parameters include the starting random number seed, the number of particles per batch, and the number of batches to simulate. Since there are no photon tallies, the keyword "secondaryMult=0" is used so that photons are not produced nor transported.

```
read
 parameters

r
a
n
d
o
m
S
e
e
d
=8655745262010035

p
e
r
B
a
t
c
h
=18700
b
a
t
c
```

(continues on next page)

(continued from previous page)

```
n
e
u
t
r
o
n
s
n
o
P
h
o
t
o
n
s

f
i
s
s
i
o
n
M
u
l
t
=0
s
e
c
o
n
d
a
r
y
M
u
l
t
=0
end
 parameters
```

Finally, the Monaco input file is ended with

```
end
 data
end
```

Output

For the case without the xcylinder shields, the tally summaries from the main output file are reported as:

```
N
e
u
t
r
o
n
P
o
i
n
t
D
e
t
e
c
t
o
r 2
.
e
x
a
m
p
l
e
p
o
i
n
t
d
e
t
e
c
t
o
r

a
v
e
r
a
g
e
s
t
a
n
d
a
r
d
e
r
r
e
l
a
```

(continues on next page)

(continued from previous page)

```
t
a
l
l
y
/
q
u
a
n
t
i
t
y
v
a
l
u
e
d
e
v
i
a
t
i
o
n
u
n
c
e
r
t
(
/
m
i
n
)   1 2 3 4 5 6

-
-
-
```

(continued from previous page)

```
u
n
c
o
l
l
i
d
e
d
f
l
u
x     4
.20334
E
-02  6
.81217
E
-05  0
.00162

t
o
t
a
l
f
l
u
x          1
.13349
E
+00  3
.28455
E
-03  0
.00290  1
.18
E
+04
X
X
X
X
X
X

-
-
-
```

(continued from previous page)

```
NeutronRegionTally 3.example regionally average standard relative
```

(continues on next page)

(continued from previous page)

```
t
a
l
l
y
/
q
u
a
n
t
i
t
y
v
a
l
u
e
d
e
v
i
a
t
i
o
n
u
n
c
e
r
t
(
/
m
i
n
)   1 2 3 4 5 6

-
-
-
```

(continued from previous page)

```
t
o
t
a
l
f
l
u
x
(
t
l
)     1
.00584
E
+00  1
.47136
E
-01  0
.14628  4
.64
E
+00
-
-
-
X
X
-

t
o
t
a
l
f
l
u
x
(
c
d
)     0.00000E+00

-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
```

(continues on next page)

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Note that in this sample calculation (10 minutes), the region tally did not pass all of the statistical checks and the relative uncertainty for the region tally is very large due to the region's small size. This shows how useful a point detector tally can be in estimating fluxes for hard-to-reach locations.

For the case with the xcylinder shields in place (450 minutes), the final results were:

```
N
e
u
t
r
o
n
P
o
i
n
t
D
e
t
e
c
t
o
r 2

a
v
e
r
a
g
e
s
t
a
n
d
a
r
d
r
e
l
a
t
F
O
M
s
t
a
t
c
h
e
c
k
s
```

(continues on next page)

(continued from previous page)

```
t
a
l
l
y
/
q
u
a
n
t
i
t
y
v
a
l
u
e
d
e
v
i
a
t
i
o
n
u
n
c
e
r
t
(
/
m
i
n
)   1 2 3 4 5 6

-
-
-
```

(continued from previous page)

```
u
n
c
o
l
l
i
d
e
d
f
l
u
x     8
.37999
E
-05  1
.44384
E
-07  0
.00172

t
o
t
a
l
f
l
u
x          1
.26869
E
-01  1
.10733
E
-04  0
.00087  4
.80
E
+03
X
X
X
X
X
X

-
-
-
```

(continued from previous page)

```
NeutronRegionTally 3.
exampleregionta
lly
averagestandardre
lat
```

(continues on next page)


```
FOMs
```

(continued from previous page)

```
t
a
l
l
y
/
q
u
a
n
t
i
t
y
v
a
l
u
e
d
e
v
i
a
t
i
o
n
u
n
c
e
r
t
(
/
m
i
n
)   1 2 3 4 5 6

-
-
-
```

(continued from previous page)

```
t
o
t
a
l
f
l
u
x
(
t
l
)     1
.40236
E
-01  1
.22375
E
-02  0
.08726  4
.80
E
-01
-
-
-
X
X
-

t
o
t
a
l
f
l
u
x
(
c
d
)     0.00000E+00

-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
```

(continues on next page)

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Here again, the region tally performed very poorly, showing that very few neutrons actually crossed the tally region. The four shields make this problem very slow to converge because rare particles can arrive at the detector after paths that see different amounts of shield.

The group-wise results list in the point detector detail files from each case can be subtracted and compared to the measurements and calculations listed in [JTN+97]. The computed and measured neutron spectra seen by the detector are shown in Fig. 5.23 through Fig. 5.27 using different cross-section libraries. For each figure, the computational times for case "A", without the shields and case "B", with the shields, were 10 minutes and 90 minutes, each on a 2 GHz Linux processor. For the CE case, 100 and 900 minutes were used to reduce the statistical uncertainties. Except for the 27/19 multigroup case shown above, none of the "B" cases passed all of the statistical tests.

Fig. 5.23: Comparison of Monaco calculated results using the ENDF/B-VII.0 27n/19g library to the measured values.

5.5.3 Activation rate from a neutron howitzer

A *neutron howitzer* is a common laboratory-sized neutron source. A few curies of an alpha emitter is mixed with an isotope that has a large (,n) cross section. This source is then stored in a large tank of moderating material (water, paraffin, etc.) with an access port. Materials can be placed into the access port for irradiation. Activation studies are a typical use of a neutron howitzer. Note that the large moderator tank also provides shielding for the users. Typical source strengths are such that users would probably not wish to spend large amounts of time in front of an open access port.

A typical size and shape for a neutron howitzer is an upright cylinder, outer radius of 30 cm by 70 cm in height. The outer wall, top, and bottom are made of 2 cm thick Plexiglas. The access port is a cylinder of radius 2 cm extending 5 cm away from the tank center through the side wall. A Plexiglas rod can be removed/inserted into the port for sample loading. The tank is filled with ordinary water. Fig. 5.28 shows a cutaway view of a very simplified model of the tank with the Plexiglas rod inserted into the access port, to prevent neutrons from streaming into the room. The source is located in the center of the tank and is small enough to be considered a point source. A small foil (1×1×0.001 cm) gold foil ^{197}Au is included as an activation sample.

Fig. 5.24: Comparison of Monaco calculated results using the ENDF/B-VII.0 200n/47g library to the measured values.

Fig. 5.25: Comparison of Monaco calculated results using the ENDF/B-V 238n library to the measured values.

Fig. 5.26: Comparison of Monaco calculated results using the ENDF/B-V 252n library to the measured values.

Fig. 5.27: Comparison of Monaco calculated results using the ENDF/B-VII CE n/p library (binned using the 200n group structure) to the measured values.

The goal is to use Monaco to calculate the activation rate density, R, in units of /cm ^{3}/s, of the gold foil

$$R = \int \Sigma\left(E\right)\phi\left(E\right)dE \tag{5.23}$$

so that the activity, A, can be calculated as a function of time in the howitzer, T, and time outside the howitzer, t. Note that the half-life of ^{198}Au of 2.7 days (decay constant is λ=2.97×10^{-6} /s).

$$A = RV\left(1 - e^{-\lambda T}\right)e^{-\lambda t} \tag{5.24}$$

Fig. 5.28: Idealized geometry for a neutron howitzer.

Input file

The following input file represents the simple model of a neutron howitzer used for a gold foil activation experiment. The file `monaco.howitzer.inp` is located in the SCALE `samples\input` directory. CSAS-MG is used to generate the cross sections.

```
'==============================================================================
' Generate the Cross Sections
'==============================================================================
=csas-mg

M
a
t
e
r
i
a
l
s
f
o
r
M
o
n
a
```

(continues on next page)

(continued from previous page)

```
v7
-27
n19
g
read
 composition

h2
o          1 1
.0 293
.0 end

p
l
e
x
i
g
l
a
s
s   2 1
.0 293
.0 end

A
u           3 1
.0 293
.0 end
end
 composition
end


'==============================================================================
' Monaco functional module and title
'==============================================================================
=monaco

M
o
n
a
c
o
/
M
A
V
R
I
C
T
r
a
i
n
i
n
g
-
E
x
```

(continues on next page)

(continued from previous page)

```
'------------------------------------------------------------------------------
' Cross Section Information
'------------------------------------------------------------------------------
read
 crossSections

a
m
p
x
F
i
l
e
U
n
i
t
=4

m
i
x
t
u
r
e 1

e
l
e
m
e
n
t   1001 6.675146E-02

e
l
e
m
e
n
t   8016 3.337573E-02
    end
 mixture

m
i
x
t
u
r
e 2

e
l
e
m
e
n
t   1001 5.678730E-02
```

(continues on next page)

(continued from previous page)

```
e
l
e
m
e
n
t   6000 3.549206E-02

e
l
e
m
e
n
t   8016 1.419682E-02
    end
 mixture

m
i
x
t
u
r
e 3

e
l
e
m
e
n
t  79197 5.772470E-02
    end
 mixture
end
 crossSections

'-------------------------------------------------------------------------------
' Geometry Block - SCALE standard geometry package (SGGP)
'-------------------------------------------------------------------------------
read
 geometry

g
l
o
b
a
l
u
n
i
t  1

c
y
l
i
n
d
e
r  1  30    35
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r  2  28    33
-33

x
c
y
l
i
n
d
e
r 3   2    30  10

x
c
y
l
i
n
d
e
r 4   2    10   5

c
u
b
o
i
d   11   7
.501 7
.500  0
.5
-0
.5  0
.5
-0
.5


m
e
d
i
a  1 1   2
-3
-4

m
e
d
i
a  2 1   1
-2
-3
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  2 1   3

m
e
d
i
a  0 1   4
-11


c
o
m
="gold foil"

m
e
d
i
a  3 1   11
v
o
l
=0
.001

b
o
u
n
d
a
r
y 4
end
 geometry


'-------------------------------------------------------------------------------
' Definitions Block
'-------------------------------------------------------------------------------
read
 definitions

r
e
s
p
o
n
s
e 1
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="gold macro"

m
a
t
=3
Z
A
I
D
=79197
M
T
=102
m
a
c
r
o

m
a
k
e
C
h
a
r
t
    end
 response


d
i
s
t
r
i
b
u
t
i
o
n 1

t
i
t
l
e
="Pu-Be Source Energy Spectra - from Knoll (Anderson & Neff)"
```

(continues on next page)

(continued from previous page)

```
a
b
s
c
i
s
s
a 11
.0
E
+06 10
.5
E
+06 10
.0
E
+06  9
.5
E
+06  9.0E+06
                  8
.5
E
+06  8
.0
E
+06  7
.5
E
+06  7
.0
E
+06  6.5E+06
                  6
.0
E
+06  5
.5
E
+06  5
.0
E
+06  4
.5
E
+06  4.0E+06
                  3
.5
E
+06  3
.0
E
+06  2
.5
E
+06  2
```

(continues on next page)

```
.0
E
+06  1.5E+06
```

(continued from previous page)

```
                    1
.0
E
+06  0
.5
E
+06  0
.0
E
+06  end

t
r
u
e
P
D
F 2
.74935
E
-03 7
.94257
E
-03 1
.38995
E
-02 8
.70628
E
-03 1.40522E-02
                  3
.37559
E
-02 4
.13930
E
-02 3
.54361
E
-02 4
.12403
E
-02 2.93264E-02
                  3
.89491
E
-02 5
.97220
E
-02 6
.76646
E
-02 6
.56789
E
-02 6.41515E-02
                  8
```

(continues on next page)

```
.11059
E
-02 6
.00275
E
-02 5
.59035
```

(continued from previous page)

```
                 8
.20223
E
-02 9
.05758
E
-02 end

r
u
n
S
a
m
p
l
e
T
e
s
t
    end
 distribution
end
 definitions

'------------------------------------------------------------------------------
' Sources Block
'------------------------------------------------------------------------------
read
 sources

s
r
c 1

n
e
u
t
r
o
n
s
s
t
r
e
n
g
t
h=1.377E+07

c
u
b
o
i
d  0 0  0 0  0 0
```

(continues on next page)

(continued from previous page)

```
e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources

'-----------------------------------------------------------------------------
' Tallies Block
'-----------------------------------------------------------------------------
read
 tallies

r
e
g
i
o
n
T
a
l
l
y 1

n
e
u
t
r
o
n

u
n
i
t
=1
r
e
g
i
o
n
=5
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e
I
D
=1
    end
 regionTally
end
 tallies

'-------------------------------------------------------------------------------
' Parameters Block
'-------------------------------------------------------------------------------
read
 parameters

r
a
n
d
o
m
S
e
e
d
= 8650005740006085

p
e
r
B
a
t
c
h
=47000
b
a
t
c
h
e
s
=10

n
e
u
t
r
o
n
s
n
o
P
```

(continues on next page)

(continued from previous page)

```
f
i
s
s
i
o
n
M
u
l
t
=0
s
e
c
o
n
d
a
r
y
M
u
l
t
=0
end
 parameters

end
 data
end
```

Output

The main text output file results are reported as:

```
N
e
u
t
r
o
n
R
e
g
i
o
n
T
a
l
l
y 1
.

a
v
e
r
a
g
e
s
t
a
n
d
a
r
d
r
e
l
a
t
F
O
M
s
t
a
t
c
h
e
c
k
s

t
a
l
l
y
/
q
u
a
n
```

(continues on next page)

(continued from previous page)

(continues on next page)

(continued from previous page)

```
t
o
t
a
l
f
l
u
x
(
t
l
)      8
.59999
E
+04   2
.64821
E
+03   0
.03079   9
.70
E
+01
X
-
X
-
X
-

t
o
t
a
l
f
l
u
x
(
c
d
)      1
.23288
E
+05   8
.52974
E
+04   0
.69186   1
.92
E
-01
-
-
-
-
-
-
```

(continues on next page)

(continued from previous page)

```
r
e
s
p
o
n
s
e 1          2
.66771
E
+05  1
.12525
E
+04  0
.04218  5
.17
E
+01
-
-
X
X
X
-

-
-
-
```

(continued from previous page)

In addition to the main output file, the diagnostics from the definitions block are shown in Fig. 5.29 and Fig. 5.30 The final value for the activation rate density R is 2.65×10^5 /cm:sup:*3*/sec. Note how the track length tally performs better than the collision density estimate for this thin foil region. But also note that after ten minutes, not all of the statistical checks are converged. Running this problem for longer times (even up to 10 hours) does not make all of the tests pass. Due to the very thin width of the of the tally region, most track-lengths across are very small but occasionally a very long track-length is recorded. This rare but high-value score tends to upset the convergence metrics. A tally region over a larger, more cuboid-like volume would make for a better behaved tally.

Fig. 5.29: Response 1.

Fig. 5.30: Distribution 1.

5.5.4 Graphite shielding measurements

K. Ueki of the Nuclear Technology Division, Ship Research Division in Japan performed many simple studies on a variety of shielding materials layered in different combinations. He and his colleagues used both neutron (^{252}Cf) and photon (^{60}Co) sources to investigate the shielding effectiveness of steel, graphite, and many hydrogen-containing materials as single shields or in combinations.

One such series of measurements was for pure graphite [UOA92] A ^{252}Cf neutron source was placed in the center of a 50 cm cube of paraffin which had a 45° cone cut-out. A neutron meter was placed 110 cm from the source. Sheets of material, in 5×80×80 cm slabs, were placed between the source and detector, with the detector side of the shield always fixed at 90 cm from the source. The shield thickness was increased on the source side of the shield. His results (read from a plot) for different thicknesses of graphite are shown in Table 5.24.

Table 5.24: Ueki's experimental results

Thickness (cm)	Dose equivalent attenuation
2	0.828810
5	0.721721
10	0.526054
15	0.364949
20	0.253182
25	0.170514
30	0.112591
35	0.074181

Input file

The following is a listing of the file monaco.graphite.inp located in the SCALE samplesinput directory. This represents a simple model of Ueki's experiment for the 20 cm graphite slab.

```
'==============================================================================
' Generate the Cross Sections
'==============================================================================
=csas-mg

M
a
t
e
r
i
a
l
s
f
o
r
M
o
n
a
c
o
/
M
A
V
R
I
C
T
r
a
i
n
i
n
g
-
E
x
e
r
c
i
```

(continues on next page)

(continued from previous page)

```
v7
-200
n47
g
read
 composition

p
a
r
a
(
h2
o
)    1          1
.0 293
.0 end

c
a
r
b
o
n       2
d
e
n
=1
.7 1
.0 300
.0 end

a
c
t
i
v
i
t
i
e
s  99          1
.0 293
.0 end
end
 composition
end


'==============================================================================
' Monaco functional module and title
'==============================================================================
=monaco

M
o
n
a
c
o
/
M
A
```

(continues on next page)

(continued from previous page)

```
'------------------------------------------------------------------------------
' Cross Section Information
'------------------------------------------------------------------------------
read
 crossSections

a
m
p
x
F
i
l
e
U
n
i
t
=4

m
i
x
t
u
r
e 1

e
l
e
m
e
n
t  1001 7.991204E-02

e
l
e
m
e
n
t  6000 3.841925E-02
    end
 mixture

m
i
x
t
u
r
e 2

e
l
e
m
e
n
t  6000 8.523484E-02
```

(continues on next page)

(continued from previous page)

```
    end
 mixtureend
 crossSections

'------------------------------------------------------------------------------
' Geometry Block - SCALE standard geometry package (SGGP)
'------------------------------------------------------------------------------
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

c
u
b
o
i
d  1   25
.0
-25
.0  25
.0
-25
.0   25
.0
-25
.0

c
o
n
e    2  10
.35948  25
.01   0
.0 0
.0
r
o
t
a
t
e
a1
=
-90
a2
=
-90
a3
=0
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d  3   90
.0  70
.0  40
.0
-40
.0   40
.0
-40
.0

c
u
b
o
i
d 99  120
.0
-30
.0  50
.0
-50
.0   50
.0
-50
.0

m
e
d
i
a 1 1  1
-2

m
e
d
i
a 0 1  2

m
e
d
i
a 2 1  3

m
e
d
i
a 0 1  99
-1
```

(continues on next page)

```
-2
-3
```

(continued from previous page)

```
b
o
u
n
d
a
r
y 99
end
 geometry

'-----------------------------------------------------------------------------
' Geometry Plots
'-----------------------------------------------------------------------------
read
 plot

s
c
r
=
y
e
s


t
t
l
="slice through plane of z=0, whole geometry"

p
i
c
=
m
i
x
t
u
r
e

x
u
l
=
-30
.0
y
u
l
=50
.0
z
u
l
=0
.0
```

(continues on next page)

(continued from previous page)

```
x
l
r
=120
.0
y
l
r
=
-50
.0
z
l
r
=0
.0

u
a
x
=1
.0
v
a
x
=0
.0
w
a
x
=0
.0

u
d
n
=0
.0
v
d
n
=
-1
.0
w
d
n
=0
.0

n
a
x
=640
    end
```

(continues on next page)

(continued from previous page)

```
t
t
l
="slice through plane of y=0, through just the paraffin block"

p
i
c
=
m
i
x
t
u
r
e

x
u
l
=
-30
.0
y
u
l
=0
.0
z
u
l
=50
.0

x
l
r
=30
.0
y
l
r
=0
.0
z
l
r
=
-50
.0

u
a
x
=1
.0
```

(continues on next page)

```
v
a
x
=0
.0
w
a
```

(continued from previous page)

```
u
d
n
=0
.0
v
d
n
=0
.0
w
d
n
=
-1
.0

n
a
x
=640
    end


t
t
l
="slice through plane of x=0, through just the paraffin block"

p
i
c
=
m
i
x
t
u
r
e

x
u
l
=0
.0
y
u
l
=
-50
.0
z
u
l
=50
.0
```

(continues on next page)

(continued from previous page)

```
x
l
r
=0
.0
y
l
r
=50
.0
z
l
r
=
-50
.0

u
a
x
=0
.0
v
a
x
=1
.0
w
a
x
=0
.0

u
d
n
=0
.0
v
d
n
=0
.0
w
d
n
=
-1
.0

n
a
x
=640
    end
end
 plot
```

(continues on next page)

(continued from previous page)

```
'-------------------------------------------------------------------------------
' Definitions Block
'-------------------------------------------------------------------------------
read
 definitions

l
o
c
a
t
i
o
n 1

p
o
s
i
t
i
o
n 110 0 0
    end
 location

r
e
s
p
o
n
s
e 5

t
i
t
l
e
="ANSI standard (1977) neutron flux-to-dose-rate factors"

s
p
e
c
i
a
l
D
o
s
e
=9029
    end
 response
```

(continues on next page)

(continued from previous page)

```
d
i
s
t
r
i
b
u
t
i
o
n 1

t
i
t
l
e
="Cf-252 neutrons, Watt spectrum a=1.025 MeV and b=2.926/MeV"

s
p
e
c
i
a
l
="wattSpectrum"

p
a
r
a
m
e
t
e
r
s 1
.025 2
.926 end
    end
 distribution
end
 definitions

'-----------------------------------------------------------------------------
' Sources Block
'-----------------------------------------------------------------------------
read
 sources

s
r
c 1
```

(continues on next page)

```
t
i
t
l
e
="Cf-252 neutrons"
```

(continued from previous page)

```
n
e
u
t
r
o
n
s
s
t
r
e
n
g
t
h=4.05E+07

c
u
b
o
i
d  0
.01 0
.01  0 0  0 0

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources

'-----------------------------------------------------------------------------
' Tallies Block
'-----------------------------------------------------------------------------
read
 tallies

p
o
i
n
t
D
e
t
e
c
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="center of detector"

n
e
u
t
r
o
n

l
o
c
a
t
i
o
n
I
D
=1

r
e
s
p
o
n
s
e
I
D
=5
    end
 pointDetector
end
 tallies

'-----------------------------------------------------------------------------
' Parameters Block
'-----------------------------------------------------------------------------
read
 parameters

r
a
n
d
o
m
S
e
e
d
=00003
e
c
d7
```

(continues on next page)

(continued from previous page)

```
p
e
r
B
a
t
c
h
=9500
b
a
t
c
h
e
s
=20

n
e
u
t
r
o
n
s
n
o
P
h
o
t
o
n
s

f
i
s
s
i
o
n
M
u
l
t
=0
s
e
c
o
n
d
a
r
y
M
u
l
t
=0
```

(continues on next page)

(continued from previous page)

```
end
 parameters

end
 data
end
```

Output

For the 20 cm case, Monaco reports the following results:

```
N
e
u
t
r
o
n
P
o
i
n
t
D
e
t
e
c
t
o
r 1
.
c
e
n
t
e
r
o
f
d
e
t
e
c
t
o
r

a
v
e
r
a
g
e
s
t
a
n
d
a
```

(continues on next page)

(continued from previous page)

```
t
a
l
l
y
/
q
u
a
n
t
i
t
y
v
a
l
u
e
d
e
v
i
a
t
i
o
n
u
n
c
e
r
t
(
/
m
i
n
)   1 2 3 4 5 6

-
-
-
```

(continued from previous page)

```
u
n
c
o
l
l
i
d
e
d
f
l
u
x     1
.06273
E
+01  2
.56481
E
-02  0
.00241

t
o
t
a
l
f
l
u
x          2
.43530
E
+02  4
.58843
E
+00  0
.01884  1
.39
E
+02
X
X
X
X
X
X

r
e
s
p
o
n
s
e 5          1
.30398
E
-02  2
.58938
E
-04  0
.01986  1
```

(continues on next page)

(continued from previous page)

(continues on next page)

(continued from previous page)

The plots generated by the "read plots" block are shown in Fig. 5.31

To compute the attenuation that Ueki measured, this dose rate can be divided by the dose rate from another Monaco calculation using a slab thickness of 0 cm—the unattenuated case. Combining the results of nine Monaco runs (eight different thicknesses and the unattenuated case), which were allowed to run long enough to achieve 1% uncertainty, gives the results shown in Table 5.25. Note how the runtime of the Monaco calculation increases with increasing shield thickness.

Fig. 5.31: Images (*.png files) generated with the "read plot" block.

Table 5.25: Measured and calculated dose attenuation rate for graphite

Thickness	Ueki		Monaco		C/E
(cm)	et al.	minutes	value	rel unc	
2	0.8288	10	0.8679	0.0072	1.05
5	0.7217	20	0.7383	0.0086	1.02
10	0.5261	40	0.5387	0.0086	1.02
15	0.3649	60	0.3837	0.0089	1.05
20	0.2532	20	0.2593	0.0199	1.02
25	0.1705	120	0.1774	0.0095	1.04
30	0.1126	180	0.1206	0.0093	1.07
35	0.0742	300	0.0806	0.0088	1.09

Adding a mesh tally

```
read
 definitions

...

g
r
i
d
G
e
o
m
e
t
r
y 7

t
i
t
l
e
="large meshes in paraffin, 5 cm mesh for shield thicknesses"

x
L
i
n
e
a
r 5
-25 25

x
L
i
n
e
a
r 12 30 90

x
p
l
a
n
e
s 100 110 120
-30 end

y
p
l
a
n
e
s
```

(continues on next page)

```
-50
-40 40 50 end
```

(continued from previous page)

```
y
L
i
n
e
a
r 7
-35 35

z
p
l
a
n
e
s
-50
-40 40 50 end

z
L
i
n
e
a
r 7
-35 35
    end
 gridGeometry
end
 definitions

read
 tallies

...


m
e
s
h
T
a
l
l
y 1

t
i
t
l
e
="example mesh tally"

n
e
u
t
r
o
n
```

(continues on next page)

(continued from previous page)

```
g
r
i
d
G
e
o
m
e
t
r
y
I
D
=7

r
e
s
p
o
n
s
e
I
D
=5

n
o
G
r
o
u
p
F
l
u
x
e
s
    end
 meshTally
end
 tallies
```

and viewing the resulting *.3dmap file with the Mesh File Viewer can produce the image shown in Fig. 5.32.

Fig. 5.32: Mesh tally showing neutron dose rate (rem/hr)

5.5.5 Simple shielding demonstration with line spectra

Sources containing line data are difficult to represent in multigroup. Comparing real measurements of line data to multigroup calculations is also difficult. This sample problem is not the simulation of a real measurement but is just a simple demonstration of the differences between continuous-energy simulation and the multigroup approach.

Consider an isotropic cobalt-60 source on one side of a slab of tungsten (5 cm thick) and the goal is to compute the photon flux and dose on the other side of the slab. Since the continuous-energy library does not have a built-in structure that could be used by tallies, the user needs to supply one (otherwise tally information is recorded in one bin covering the entire range of energy). The user can construct an energy boundaries object in the definitions block that is uniformly spaced, logarithmically spaced, based on one of the multigroup libraries or any combination of the above.

Input file

The sample problem `monaco.wSlab.inp`, is located in the `samples\input` directory. The materials input consist just of tungsten, in its natural isotopic abundances.

```
read
 crossSections

c
e
L
i
b
r
a
r
y
="ce_v7.1_endf.xml"

m
i
x
t
u
r
e 1
```

(continues on next page)

(continued from previous page)

```
e
l
e
m
e
n
t  74182 1.531781E-02

e
l
e
m
e
n
t  74183 8.202875E-03

e
l
e
m
e
n
t  74184 1.806470E-02

e
l
e
m
e
n
t  74186 1.671717E-02
    end
 mixture
end
 crossSections
```

The geometry is a simple slab of tungsten, with a small air region on one side for a region tally.

```
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

c
u
b
o
i
d 10   2
.5
.2
.5  25
.0
-25
```

(continues on next page)

(continued from previous page)

```
                                   25
.0
-25
.0

c
u
b
o
i
d 20   6
.0   4
.0   1
.0
-1
.0
                                    1
.0
-1
.0

c
u
b
o
i
d 30  10
.0
-10
.0  25
.0
-25
.0
                                   25
.0
-25
.0


m
e
d
i
a 1 1  10

m
e
d
i
a 0 1  20
v
o
l
=8
.0

m
e
d
i
a 0 1  30
-10
-20
```

(continues on next page)

(continued from previous page)

```
b
o
u
n
d
a
r
y 30
end
 geometry
```

Fig. 5.33: Simple slab geometry with a source (S) on the left and a tally region (T) on the right.

In the definitions block, a location (for a point detector), the photon dose response function, the Co-60 line spectra and an energy boundaries structure are all defined. The energyBounds defined here has a base structure of 30 bins that are 50 keV wide, with three bins that are 2 keV wide at the cobalt line energies and the 511 keV annihilation gamma energy.

```
read
 definitions

l
o
c
a
t
i
o
n 1
```

(continues on next page)

(continued from previous page)

```
p
o
s
i
t
i
o
n 5
.0 0
.0 0
.0
    end
 location


r
e
s
p
o
n
s
e 5

t
i
t
l
e
="ANSI standard (1977) photon flux-to-dose-rate factors"

d
o
s
e
D
a
t
a
=9504
    end
 response


d
i
s
t
r
i
b
u
t
i
o
n 1
```

(continues on next page)

(continued from previous page)

```
t
i
t
l
e
="cobalt-60 gammas/decay"

d
i
s
c
r
e
t
e   347140   826100 1173228 1332492  2158570    2505692 end

t
r
u
e
p
d
f  0
.000075 0
.000076 0
.9985 0
.999826 0
.000012 0
.00000002 end
    end
 distribution



e
n
e
r
g
y
B
o
u
n
d
s 1

l
i
n
e
a
r 30 0
.00
e6 1.50e6

b
o
u
n
d
s  0
.510
```

(continues on next page)

(continued from previous page)

```
    end
 energyBounds
end
 definitions
```

The source is a simple point source 5 cm to the left of the slab. Because the distribution of cobalt gamma rays was entered as gammas per decay, the keyword 'useNormConst' will set the source strength to be the total of the energy distribution - about 2 photons/decay. The 'multiplier'keyword is used to multiply that strength by 37×10^9 decays/sec to get 1 Ci.

```
read
 sources

s
r
c 1

t
i
t
l
e
="one Ci of cobalt-60"

u
s
e
N
o
r
m
C
o
n
s
t

m
u
l
t
i
p
l
i
e
r=37e9

s
p
h
e
r
e 0
.0
o
r
i
g
i
n
x
=
-5
```

(continues on next page)

(continued from previous page)

```
p
h
o
t
o
n
s

e
D
i
s
t
r
i
b
u
t
i
o
n
I
D
=1
    end
 src
end
 sources
```

Both a region tally and a point detector tally are defined. Parameters are set for a 10 minute calculation.

```
read
 tallies

p
o
i
n
t
D
e
t
e
c
t
o
r 15

p
h
o
t
o
n

l
o
c
a
t
i
o
n
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```
r
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s
p
o
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s
e
I
D
=5

e
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y
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u
n
d
s
I
D
=1
    end
 pointDetector

r
e
g
i
o
n
T
a
l
l
y 24

p
h
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u
n
i
t
=1
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(continues on next page)

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r
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s
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    end
 regionTally
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read
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a
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b4
e3
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n
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s
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M
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t
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Output

Results for the dose rate from this continuous-energy calculation are shown in Table 5.26, along with results from two multigroup calculations and an MCNP calculation. To simulate the same type of physics used in the continuous-energy SCALE, the MCNP calculation used a photon cutoff energy of 0.01 MeV, EMCPF=100 MeV (detailed physics), IDES=1 (no electrons/no bremsstrahlung), NOCOH=0 (coherent scattering occurs), ISPN=0 (no photonuclear collisions), and NODOP=1 (no Doppler energy broadening).

The results from the SCALE multigroup calculations differ by 20%, due to how the source and the dose response function are represented. The 19-group structure represents the 1.33 MeV line with the 1.33-1.66 MeV, so it is expected that the computed dose will be high. With the 47-group structure, the 1.17 MeV line is represented by the 1-1.2 MeV group (too low – lower dose will result) and the 1.33 MeV line is represented by the 1.33-1.44 MeV group (too high – higher dose will result). The multigroup results are well-converged – just not as accurate as desired. The continuous-energy results should be more accurate.

Table 5.26: Dose rates for the cobalt-60/tungsten problem using different energy treatments.

	Time	Point Detector		Region Tally	
	(min)	rem/hr	rel unc	rem/hr	rel unc
MCNP	97.8	3.1088	0.0039	3.1376	0.0051
SCALE CE	89.9	3.1886	0.0027	3.0949	0.0136
SCALE 47	89.9	2.9284	0.0012	3.0144	0.0077
SCALE 19	90.0	3.6705	0.0010	3.7414	0.0065

Fig. 5.34 and Fig. 5.35 show the results of the point detector and region tally flux as a function of energy, for this problem as well as two multigroup calculations and an MCNP calculation. Tables M and N list the flux values of the cobalt lines and the annihilation gamma for the two tally types.

Fig. 5.34: Point detector fluxes for the cobalt-60/tungsten problem using different energy treatments.

Fig. 5.35: Region tally fluxes for the cobalt-60/tungsten problem using different energy treatments.

Table 5.27: Region tally fluxes for the cobalt-60/tungsten problem using different energy treatments.

	511000 eV		1173230 eV		1332490 eV	
	/cm^2/s	rel unc	/cm^2/s	rel unc	/cm^2/s	rel unc
MCNP	1.91E+00	0.0320	9.53E+01	0.0125	1.41E+02	0.0093
SCALE CE	2.02E+00	0.0382	9.94E+01	0.0058	1.42E+02	0.0041
SCALE 47	2.31E+00	0.0149				
SCALE 19						

Table 5.28: Region tally flux values for the lines.

	511000 eV		1173230 eV		1332490 eV	
	/cm^2/s	rel unc	/cm^2/s	rel unc	/cm^2/s	rel unc
MCNP	2.15E+00	0.0945	9.60E+01	0.0145	1.44E+02	0.0118
SCALE CE	2.58E+00	0.2231	1.01E+02	0.0402	1.38E+02	0.0345
SCALE 47	2.55E+00	0.1200				
SCALE 19						

CHAPTER

SIX

CRITICALITY SAFETY OVERVIEW

Introduction by B. T. Rearden

SCALE provides a suite of computational tools for criticality safety analysis that is primarily based on the KENO Monte Carlo code for eigenvalue neutronics calculations [GPJD+11]. Two variants of KENO provide identical solution capabilities with different geometry packages. KENO V.a uses a simple and efficient geometry package sufficient for modeling many systems of interest to criticality safety and reactor physics analysts. KENO-VI uses the SCALE Generalized Geometry Package, which provides a quadratic-based geometry system with much greater flexibility in problem modeling but with slower runtimes. Both versions of KENO perform eigenvalue calculations for neutron transport primarily to calculate multiplication factors (*keff*) and flux distributions of fissile systems in both continuous energy and multigroup modes. They are typically accessed through the integrated SCALE sequences described below. KENO's grid geometry capability extends region-based features for accumulating data for source or biasing parameter specifications, as well as for tallying results from a calculation for visualization or communication of data into or out of a calculation. Criticality safety analysts may also be interested in the sensitivity and uncertainty analysis techniques that can be applied for code and data validation as described elsewhere in this document.

Criticality Safety Analysis Sequences

The Criticality Safety Analysis Sequences (CSAS) with KENO V.a (CSAS5) and KENO-VI (CSAS6**)** provide a reliable, efficient means of performing *keff* calculations for systems routinely encountered in engineering practice. The CSAS sequences implement XSProc to process material input and provide a temperature and resonance-corrected cross section library based on the physical characteristics of the problem being analyzed. If a continuous energy cross section library is specified, no resonance processing is needed, and the continuous energy cross sections are used directly in KENO, with temperature corrections provided as the cross sections are loaded.

A search capability is available with CSAS5 to find desired values of *keff* as a function of dimensions or densities. The two basic search options offered are (1) an optimum search seeking a maximum or minimum value of *keff* and (2) a critical search seeking a fixed value of *keff*.

For continuous energy calculations, reaction rate tallies can be requested within the CSAS input, and for multigroup calculations, reaction rate calculations are performed using the KENO Module for Activity-Reaction Rate Tabulation (KMART) post-processing tools. A conversion tool is provided to up-convert KENO V.a input to KENO-VI either as a direct KENO input (K5toK6) or, more commonly, as a CSAS sequence (C5toC6).

STARBUCS: Burnup-Credit Analysis Sequence

The Standardized Analysis of Reactivity for Burnup Credit using SCALE (STARBUCS) [GB01][RG09] is a control module to perform criticality calculations for spent fuel systems employing burnup credit. STARBUCS automates the criticality safety analysis of spent fuel configurations by coupling the depletion and criticality aspects of the analysis, thereby eliminating the need to manually process the spent fuel nuclide compositions into a format compatible with criticality safety codes.

STARBUCS performs a depletion analysis calculation for each spatially varying burnup region (if an axial or horizontal burnup profile is specified) of a spent fuel assembly using the ORIGEN-ARP methodology of SCALE. If a multigroup calculation is to be performed in KENO, the spent fuel compositions are then used to generate reso-

nance self-shielded cross sections for each burnup-dependent fuel region. Finally, a KENO criticality calculation is performed to determine the neutron multiplication factor for the system.

The STARBUCS input format has been designed around the existing depletion analysis and criticality safety sequences of SCALE. Only a minimal amount of input beyond that typically required for a fresh-fuel calculation is needed to perform a burnup-credit calculation.

STARBUCS was developed to facilitate studies of major burnup-credit phenomena, such as those identified in the US Nuclear Regulatory Commission's *Interim Staff Guidance 8*, [Com12] but it is restricted to modeling one assembly type with the same starting enrichment loaded throughout the transportation or storage model. Greater flexibility is available by computing individual assembly burnup compositions with the ORIGAMI code and then creating a KENO model to implement these compositions.

For burnup loading curve iterative calculations, STARBUCS employs the search algorithm from CSAS5 to determine initial fuel enrichments that satisfy a convergence criterion for the calculated *keff* value of the spent fuel configuration.

Sourcerer: Hybrid Method for Starting Source Distribution

As the fidelity of criticality models continues to increase, especially for storage and transportation systems, the ability of the Monte Carlo codes to consistently provide a converged fission source can be challenging. Studies have shown that using a starting fission distribution similar to the true fission distribution can reduce the number of skipped generations required for fission source convergence, and it can significantly improve the reliability of the final *keff* result [IPW+11]. The Sourcerer sequence applies the Denovo [ESSC10] discrete ordinates code to generate a starting fission source distribution in a KENO Monte Carlo calculation. The discrete ordinates calculation is performed on a user-defined Cartesian grid geometry where macroscopic material definitions are automatically created from the Monte Carlo model and multigroup group cross sections are appropriately generated.

For many criticality safety applications, the additional step of performing a deterministic calculation to initialize the starting fission source distribution is not necessary. However, for challenging criticality safety analyses such as as-loaded spent nuclear fuel transportation packages with a mixed loading of low- and high-burnup fuel, even a low-fidelity deterministic solution for the fission source produces more reliable results than the typical starting distributions of uniform or cosine functions over the fissionable regions, as demonstrated in a recent study [Ibr13].

Criticality Accident Alarm System Analysis with KENO and MAVRIC

Criticality accident alarm systems (CAAS) safety analyses modeling presents challenges because the analysis consists of a criticality problem and a deep-penetration shielding problem [PPJ09]. Modern codes are typically optimized to handle one of these types of problems, but not both. The two problems also differ in size—the criticality problem depends on materials relatively close to the fissionable materials, whereas the shielding problem can cover a much larger range.

CAAS analysis can be performed using the CSAS6 criticality sequence and the MAVRIC shielding sequence. First, the fission distribution (in space and energy) is determined via CSAS6. This information is collected on a grid geometry that overlies the physical geometry model and is saved as a Monaco mesh source file. The mesh source is then used as the source term in MAVRIC. The absolute source strength is set by the user to the total number of fissions (based on the total power released) during the criticality excursion. MAVRIC can be optimized to calculate a specific detector response at one location or to calculate multiple responses/locations with roughly the same relative uncertainty.

CHAPTER

SEVEN

CSAS5: CONTROL MODULE FOR ENHANCED CRITICALITY SAFETY ANALYSIS SEQUENCES WITH KENO V.A

L. M. Petrie, K. B. Bekar, S. Goluoglu, D. F. Hollenbach,* N. F. Landers*

The **C**riticality **S**afety **A**nalysis **S**equences with KENO V.a (CSAS5) provides reliable and efficient means of performing k_{eff} calculations for systems that are routinely encountered in engineering practice. In the multigroup calculation mode, CSAS5 uses XSProc to process the cross sections for temperature corrections and problem-dependent resonance self-shielding and calculates the k_{eff} of a three-dimensional (3-D) system model. If the continuous energy calculation mode is selected no resonance processing is needed and the continuous energy cross sections are used directly in KENO V.a, with temperature corrections provided as the cross sections are loaded. The geometric modeling capabilities available in KENO V.a coupled with the automated cross-section processing within the control sequences allow complex, 3-D systems to be easily analyzed. A search capability is achieved by repeatedly activating the control module MODIFY, to alter either the system dimensions or densities, and the functional module KENO V.a to calculate the k_{eff} for the modified dimensions or densities.

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7.1 Acknowledgments

CSAS5 and its related Criticality Safety Analysis Sequences are based on the old CSAS2 control module (no longer in SCALE) and the KENO V.a functional module described in the KENO V.a chapter. Therefore, special acknowledgment is made to J. A. Bucholz, R. M. Westfall, and J. R. Knight who developed CSAS2. G. E. Whitesides is acknowledged for his contributions through early versions of KENO. Appreciation is expressed to C. V. Parks and S. M. Bowman for their guidance in developing CSAS5.

Special appreciation is expressed to S. J. Poarch and S. Y. Walker for their efforts in formatting this document.

7.2 Introduction

Criticality Safety Analysis Sequence with KENO V.a (CSAS5) provides reliable and efficient means of performing k_{eff} calculations for systems that are routinely encountered in engineering practice, especially in the calculation of k_{eff} of three-dimensional (3-D) system models. CSAS5 implements XSProc to process material input and provide a temperature and resonance-corrected cross-section library based on the physical characteristics of the problem being analyzed. If a continuous energy cross-section library is specified, no resonance processing is needed and the continuous energy cross sections are used directly in KENO V.a, with temperature corrections provided as the cross sections are loaded. A search capability is available to find a desired values of k_{eff} as a function of dimensions or densities. The two basic search options offered are (1) an optimum search seeking a maximum or minimum value of k_{eff} and (2) a critical search seeking a fixed value of k_{eff}.

All the control sequences in the CSAS5 control module are listed in Table 7.1 with the modules they invoke. The first four sequences are subsets of the CSAS5 sequence.

Table 7.1: CSAS5 sequences for criticality safety

Control sequence	Function	Functional modules executed by the control sequence for multigroup libraries		
CSAS5	k_{eff} (3-D)	XSProc	KENO V.a	
CSAS5S	k_{eff} (3-D) search	XSProc	KENO V.a	MODIFY

7.3 Sequence Capabilities

In order to minimize human error, the SCALE data handling is automated as much as possible. CSAS5 and many other SCALE sequences apply a standardized procedure to provide appropriate number densities and cross sections for the calculation. XSProc is responsible for reading the standard composition data and other engineering-type specifications, including volume fraction or percent theoretical density, temperature, and isotopic distribution as well as the unit cell data. XSProc then generates number densities and related information, prepares geometry data for resonance self-shielding and flux-weighting cell calculations, if needed, and (if needed) provides problem-dependent multigroup cross-section processing. Sequences that execute KENO V.a include a KENO V.a Data Processor to read and check the KENO V.a data. Sequences that execute a search use a Search Data Processor to read and check the search data. When the data checking has been completed, the control sequence executes XSProc to prepare a resonance-corrected microscopic cross-section library in the AMPX working library format if a multigroup library has been selected.

For each unit cell specified as being cell-weighted, XSProc performs the necessary calculations and produces a cell-weighted microscopic cross-section library. KENO V.a may be executed to calculate the k_{eff} or neutron multiplication factor using the cross-section library that was prepared by the control sequence. MODIFY may be invoked to perform a search [LDPW79] by repeatedly altering the unit cell (multigroup mode only) and KENO V.a data prior to executing the next pass through the calculation. Cross sections are updated at the beginning of each search pass with the modified data. If unit cell data is altered as part of the search, i.e., pitch or material search, the cross-sections are correctly processed with the updated data.

The search capability is implemented by the control module MODIFY. It performs operations according to the specified search data to determine (1) the maximum or minimum value of k_{eff} as a function of pitch, dimensions or densities or (2) the pitch, dimensions, or densities corresponding to a specified value of k_{eff}. An iterative procedure is used, making use of all previous information to modify the dimensions or densities to achieve the desired result. The procedures for conducting optimum and critical searches are summarized in the following sections.

7.3.1 Optimum (minimum/maximum) search

Because only an initial value of k_{eff} and a set of boundary constraints are available, four initial points are generated spanning the range defined by the constraints. The search package identifies the type of cubic equation [i.e., a cubic with no local extrema (type A) or a cubic with two local extrema (type B)] and utilizes this knowledge in determining the pitch, dimensions, or material densities corresponding to the maximum (or minimum) value of k_{eff}. The optimum search procedure is summarized as follows:

1. Calculate k_{eff} for the specified problem.
2. Calculate k_{eff} for the minimum constraint.
3. Calculate k_{eff} for the maximum constraint.
4. Calculate k_{eff} for a fourth point that lies approximately equidistant between the initial guess and the constraint that is farthest from it.

5. Utilize a weighted least-squares fit to a cubic polynomial on the data points.
6. Determine the type of cubic. For a type A cubic, go to step 11.
7. Take the first derivative of the least-squares cubic.
8. Solve the quadratic for its roots.
9. Take the second derivative of the least-squares cubic to determine which root is the maximum (or minimum), and if it falls within the constraints, use this root as the next guess. Otherwise, convergence has been defined as occurring at the constraint with the maximum (or minimum) k_{eff}.
10. Calculate the k_{eff} corresponding to the next guess. Go to step 5. Repeat this procedure until convergence is achieved.
11. If the cubic equation is a type A cubic, the optimum lies on one of the boundaries. If the fit shows that the cubic is actually a type B cubic, go to step 7 and continue.

Convergence is defined as occurring when a k_{eff} has been calculated for a point on the curve where the value of the curve is within epsilon of the maximum (or minimum) of the curve. Additionally, the calculated k_{eff} must be within two standard deviations of the value of the curve at that point. The search is terminated when convergence is achieved, when the code determines there is no local maximum within the constraints, or the maximum number of search iterations is reached.

Note: At the beginning of each search pass, the cross sections are updated using the updated values of pitch, dimensions, or material densities. Also, the unit or material being modified can be directly tied to a unit cell, so that unit cell is updated during the search. Therefore, the final result should be consistent with the results obtained by running a non-search problem using the data from the last pass.

7.3.2 Critical search

The critical search option searches for the pitch, dimensions, or material densities corresponding to a specified value of k_{eff}. If the calculated value of k_{eff} is within the specified search tolerance (EPS) of the desired k_{eff}, the search is considered to be complete. The critical search procedure is summarized as follows:

1. Calculate k_{eff} for the specified problem. If it is within EPS of the specified k_{eff}, convergence has been achieved.

2. Calculate k_{eff} for one of the constraints. If the specified k_{eff} of the system does not fall between the initial value and the k_{eff} of the constraint, calculate the k_{eff} of the other constraint. If the calculated k_{eff} is within EPS of the specified k_{eff}, convergence has been achieved.

3. Calculate k_{eff} for a point chosen from a linear fit of the two existing points closest to the specified k_{eff}.

4. Repeat step 3 until convergence has been achieved, the program determines that the specified value lies outside the constraints, or the maximum number of search iterations is reached. Convergence has been achieved when the calculated **k*$_{\text{eff}}$ is within EPS of the specified k_{eff}.

5. If convergence is achieved, calculate k_{eff} for a point determined from fitting the previous points to a cubic and solving the cubic for the point closest to the desired k_{eff}. If all roots lie outside the constraints, the problem is terminated and an appropriate message is written. If the maximum number of iterations is reached without the problem converging, the problem is terminated and an appropriate message is written.

Note: At the beginning of each search pass, the cross sections are updated using the updated values of pitch, dimensions, or material densities. Also, the unit or material being modified can be directly tied to a unit cell, so that unit

cell is updated during the search. Therefore, the final result should be consistent with the results obtained by running a non-search problem using the data from the last pass.

7.3.3 Multigroup CSAS5 limitations

The CSAS5 control module was developed to use simple input data and prepare problem-dependent cross sections for use in calculating the effective neutron multiplication factor of a 3-D system using KENO V.a. An attempt was made to make the system as general as possible within the constraints of the standardized methods chosen to be used in SCALE. Standardized methods of data input were adopted to allow easy data entry and for quality assurance purposes. Some of the limitations of the CSAS5 multigroup sequences are a result of using preprocessed multigroup cross sections. Inherent limitations in multigroup CSAS5 calculations are as follows:

1. Two-dimensional (2-D) effects such as fuel rods in assemblies where some positions are filled with control rod guide tubes, burnable poison rods and/or fuel rods of different enrichments. The cross sections are processed as if the rods are in an infinite lattice of identical rods. If the user inputs a Dancoff factor for the cell (such as one computed by MCDancoff), XSProc can produce an infinite lattice cell, which reproduces that Dancoff. This can mitigate some two dimensional lattice effects

7.3.4 Continuous energy CSAS5 limitations

When continuous energy KENO calculations are desired, none of the resonance processing capabilities of XSProc are applicable or needed. The continuous energy cross sections are directly used in KENO. An existing multigroup input file can easily be converted to a continuous energy input file by simply specifying the continuous energy library. In this case, all cell data is ignored. However, the following limitations exist:

1. If CELLMIX is defined in the cell data, the problem will not run in the continuous energy mode. CELLMIX implies new mixture cross sections are generated using XSDRNPM-calculated cell fluxes and therefore is not applicable in the continuous energy mode.
2. Only VACUUM, MIRROR, PERIODIC, and WHITE boundary conditions are allowed. Other albedos, e.g., WATER, CARBON, POLY, etc. are for multigroup only.
3. Problems with DOUBLEHET cell data are not allowed as they inherently utilize CELLMIX feature.

7.4 Input Data Guide

This section describes the input data required for CSAS5. Several subsets of the CSAS5 sequences listed in Table 7.1 are available to achieve several different levels of processing.

The input data for these CSAS5 sequences are composed of three broad categories of data. The first is XSProc, including Standard Composition Specification Data and Unit Cell Geometry Specification. This first category specifies the cross-section library and defines the composition of each mixture and optionally unit cell geometry that may be used to process the cross sections. This data block is necessary for all CSAS5 sequences. The second category of data, the KENO V.a input data, is used to specify the geometric and boundary conditions that represent the physical 3-D configuration of a KENO V.a problem. Both data blocks are necessary for CSAS5 and CSAS5S. The last category of data is the search data and is required only for CSAS5S.

All data are entered in free form, allowing alphanumeric data, floating-point data, and integer data to be entered in an unstructured manner. Up to 252 columns of data entry per line are allowed. Data can usually start or end in any column with a few exceptions. As an example, the word END beginning in column 1 and followed by two blank spaces or a new line will end the problem and any data following will be ignored. Each data entry must be followed by one or more blanks to terminate the data entry. For numeric data, either a comma or a blank can be used to terminate each data entry. Integers may be entered for floating-point values. For example, 10 will be interpreted as 10.0. Imbedded blanks

are not allowed within a data entry unless an E precedes a single blank as in an unsigned exponent in a floating-point number. For example, 1.0E 4 would be correctly interpreted as 1.0×10^4.

The word "END" is a special data item. An "END" may have a name or label associated with it (e.g., "END DATA"). The name or label associated with an "END" is separated from the "END" by a single blank and is a maximum of 12 characters long. *At least two blanks or a new line MUST follow every labeled and unlabeled "END." It is the user's responsibility to ensure compliance with this restriction. Failure to observe this restriction can result in the use of incorrect or incomplete data without the benefit of warning or error messages.*

Multiple entries of the same data value can be achieved by specifying the number of times the data value is to be entered, followed by either R, *, or $, followed by the data value to be repeated. Imbedded blanks are not allowed between the number of repeats and the repeat flag. For example, 5R12, 5*12, 5$12, or 5R 12, etc., will enter five successive 12s in the input data. Multiple zeros can be specified as nZ where n is the number of zeroes to be entered.

The purpose of this section is to define the input data in discrete subsections relating to a particular type of data. Tables of the input data are included in each subsection, and the entries are described in more detail in the appropriate sections.

Resonance-corrected cross sections are generated using the appropriate boundary conditions for the unit cell description (i.e., void for the outer surface of a single unit, white for the outer surface of an infinite array of cylinders). As many unit cells as needed may be specified in a problem. A unit cell is cell-weighted by using the keyword "CELLMIX=" followed by a unique user specified mixture number in the unit cell data.

To check the input data without actually processing the cross sections, the words "PARM=CHECK" or "PARM=CHK" should be entered, as shown below.

```
=CSAS5 PARM=CHK
or
#CSAS5 PARM=CHK
```

This will cause the input data for CSAS5 to be checked and appropriate error messages to be printed. If plots are specified in the data, they will be printed. This feature allows the user to debug and verify the input data while using a minimum of computer time.

7.4.1 XSProc data

The XSProc reads the standard composition specification data and the unit cell geometry specifications. It then produces the mixing table and unit cell information necessary for processing the cross sections if needed. The XSProc section of this manual provides a detailed description of the input data and processing options.

7.4.2 KENO V.a data

If the problem utilizes a sequence that contains KENO V.a as a functional module, the input to KENO V.a comes after the XSProc input. Table 7.2 contains the outline for the KENO V.a input and the SEARCH input, which is required for a search case (i.e., CSAS5S). The KENO V.a input is divided into 13 data blocks and CSAS5S includes an additional block of search data. A brief outline of commonly used data blocks is shown in Table 7.2. Note that parameter data must precede all other KENO data blocks. Information on all KENO V.a input is provided in the KENO chapter of this document and will not be repeated here.

Table 7.2: Outline of KENO data

Type of data	Starting flag	Comments	Termination flag
Parameters*	READ PARAMETER	Enter desired parameter data	END PARAMETER
Geometry	READ GEOMETRY	Enter desired geometry data	END GEOMETRY
Array data	READ ARRAY	Enter desired array data	END ARRAY
Boundary conditions	READ BOUNDS	Enter desired boundary conditions	END BOUNDS
Energy group boundaries	READ ENERGY	Enter desired neutron energy group boundaries	END ENERGY
Start data or initial source	READ START	Enter desired start data	END START
Plot data	READ PLOT	Enter desired plot data	END PLOT
Grid geometry data	READ GRID	Enter desired mesh data	END GRID
Reaction	READ REACTION	Enter desire reaction tallies (CE mode only)	END REACTION
KENO V.a data terminus	END DATA	Enter to signal the end of all KENO V.a data	
Search data	READ SEARCH	Enter for CSAS5	END SEARCH
*Must precede all other data blocks in this table.			

7.4.3 Search data

Search data must be entered for CSAS5S. The search data enable the code to perform a search according to the instructions specified by the user. The code begins reading search data when it encounters the words READ SEARCH and continues reading search data until it encounters the words END SEARCH. Search data consist of the search type specification and auxiliary search commands.

Search type specification

These data are used to define the type of search and to set the parameters that provide limits for the search. The search type specification data consist of (a) a search descriptor, (b) the search type, and (c) optional search parameters as described below.

SEARCH DESCRIPTOR is used to define the search mode.

Use OPTIMUM if the maximum value of k_{eff} is to be determined.

Use CRITICAL if a specified value of k_{eff} is to be obtained.

Use MINIMUM if the minimum value of k_{eff} is to be determined.

SEARCH TYPE is used to specify the variable that is to be changed during the search procedure.

Use PITCH to alter the center-to-center spacing between the units at the lowest array level. By default only the spacing in the X and Y directions will be altered. Use DIMENSION to alter the dimensions of one or more geometry regions in one or more units. Use CONCENTRATION to alter the concentration of one or more standard compositions in one or more mixtures.

The combination of the search descriptor and the search type defines the search method. Each search type has a set of predefined defaults and the ability to change the default settings and expand the scope of the search. Only one SEARCH DESCRIPTOR and one SEARCH TYPE are allowed in a problem.

An OPTIMUM PITCH search determines the pitch that gives the maximum value of k_{eff}.* By default the X spacing will be altered for slab arrays, the X and Y spacing will be altered for arrays of cylinders, and the X, Y, and Z spacing will be altered for spherical arrays. Auxiliary search commands can be used to instruct the code to change any of these defaults.

An OPTIMUM DIMENSION search determines the maximum value of k_{eff} by altering the dimensions of one or more geometry regions in one or more units in accordance with the specified auxiliary search commands. Only the dimensions specified in the search commands will be modified. The relative variations in dimensions are determined by the search constants specified for each dimension.

An OPTIMUM CONCENTRATION search determines the maximum value of k_{eff} by altering the concentration of standard compositions in mixtures in accordance with specified search commands. Only the standard compositions in the materials specified are altered. The relative variations in concentrations are determined by the search constants specified for each composition.

A CRITICAL PITCH search alters the spacing between units in the same manner as an optimum pitch search to achieve the specified value of k_{eff}. By default the X spacing will be altered for slab arrays, the X and Y spacing will be altered for arrays of cylinders, and the X, Y, and Z spacing will be altered for spherical arrays. Auxiliary search commands can be used to instruct the code to change any of these defaults.

A CRITICAL DIMENSION search alters the dimensions of one or more geometry regions in accordance with the specified auxiliary search commands to achieve the specified value of k_{eff}.* Only the dimensions specified in the search commands will be modified. The relative variations in dimensions are determined by the search constants specified for each dimension.

A CRITICAL CONCENTRATION search alters the concentration of standard compositions in mixtures in accordance with the specified auxiliary search commands to achieve the specified value of k_{eff}. Only the standard compositions in the materials specified are altered. The relative variations in concentrations are determined by the search constants specified for each composition.

A MINIMUM PITCH search determines the pitch that gives the minimum value of k_{eff}. By default the X spacing will be altered for slab arrays, the X and Y spacing will be altered for arrays of cylinders, and the X, Y, and Z spacing will be altered for spherical arrays. Auxiliary search commands can be used to instruct the code to change any of these defaults.

A MINIMUM DIMENSION search determines the minimum value of k_{eff} by altering the dimensions of one or more geometry regions in one or more units in accordance with the specified auxiliary search commands. Only the dimensions specified in the search commands will be modified. The relative variations in dimensions are determined by the search constants specified for each dimension.

A MINIMUM CONCENTRATION search determines the minimum value of k_{eff} by altering the concentration of standard compositions in mixtures in accordance with specified search commands. Only the standard compositions in the materials specified are altered. The relative variations in concentrations are determined by the search constants specified for each composition.

OPTIONAL SEARCH PARAMETERS are entered after the SEARCH DESCRIPTOR AND SEARCH TYPE and are used to alter the default values of the optional search parameters. Only one set of optional search parameters can be entered for a problem. The optional search parameters are listed below.

PAS=nn is used to set the maximum number of times the search will calculate k_{eff}.* The first pass calculates the k_{eff} corresponding to the initial geometry dimensions. The second pass calculates the k_{eff} corresponding to one of the constraints, and the third pass often corresponds to the other constraint. After the third pass, the search dimensions or concentrations are changed based on a fit to a quadratic or cubic equation. The default value of nn is 10.

NPM=nn is used to set the number of search parameters. The default value of nn is 1 and should not be overridden.

EPS=ff is used to set the search convergence tolerance (the amount by which k_{eff} is allowed to vary from the desired k_{eff}). An optimum or minimum search is terminated when the calculated k_{eff} is within EPS of the optimum or minimum value as indicated by the mathematical fit to the calculated points. A critical search is terminated when the calculated k_{eff} is within EPS of the specified k_{eff}. The default value of ff is 0.005.

KEF=ff is used only for a CRITICAL search. The default value of ff is 1.000.

MINPITCH=ff is allowed ONLY for a PITCH search. It is used to specify the minimum allowed pitch (center-to-center spacing in the X; X,Y; or X,Y,Z directions depending on array type) between the units in an array. The search will terminate if the pitch becomes smaller than the specified minimum pitch. The default value of ff is the pitch at which the region immediately inside the outer most region of the unit touches the same region in an adjacent unit. It is much easier to specify the minimum allowed pitch than to calculate the appropriate value of the minimum constraint.

MAXPITCH=ff is allowed ONLY for a PITCH search. It is used to specify the maximum allowed pitch (center-to-center spacing in the X; X, Y; or X, Y, Z directions depending on array type) between units in an array. The search will terminate if the specified pitch is exceeded. The default value of ff is the pitch corresponding to 5 times the parameter that corresponds to the minimum pitch. It is much easier to specify a maximum allowed pitch than to calculate the appropriate value of the maximum constraint.

MORE is used to terminate the optional search parameters and initiate the auxiliary search commands. Do not enter MORE unless auxiliary search commands are to be entered. This command may only be entered once, immediately prior to the auxiliary search commands.

Table 7.3: Outline of search type specification

Entry No.	Type of data	Data entry	Comments
1	Search descriptor	OPTIMUM	Initiates a search for the maximum value of *keff*.
		CRITICAL	Initiates a search for a specified value of *keff*.
		MINIMUM	Initiates a search for the minimum value of *keff*.
2	Search type	PITCH	Vary the pitch of an array.
		DIMENSION	Vary one or more dimensions in one or more regions of one or more units.
		CONCENTRATION	Vary the concentration of one or more standard compositions in one or more mixtures.
3	Optional search parameters		Optional search parameters allow changing default values. Any or all may be entered in any order.
3a	No. of search passes	PAS=	Enter the keyword PAS= followed by the desired number of search passes. Default=10.
3b	No. of search parameters	NPM=	Enter the keyword NPM= followed by the number of search parameters. Present capability is limited to 1.
3c	Search convergence tolerance	EPS=	Enter the keyword EPS= followed by the desired convergence tolerance. Default=0.005.
3d	Desired value of *keff*	KEF=	Enter the keyword KEF= followed by the desired value of *keff*. The default value is 1.000. DO NOT ENTER FOR OPTIMUM OR MINIMUM SEARCHES.
3e	Maximum allowed pitch	MAXPITCH=	Enter the keyword MAXPITCH= followed by the maximum allowed pitch for a search whose search type, entry 2 above, is PITCH. The default value is the pitch corresponding to 5.0 times the parameter at the minimum possible pitch.
3f	Minimum allowed pitch	MINPITCH=	Enter the keyword MINPITCH= followed by the minimum allowed pitch for a search whose search type, entry 2 above, is PITCH. The default value is the minimum possible pitch (i.e., the pitch at which the shapes in the array touch).
4	Additional search data	MORE	Enter the delimiter MORE. This delimiter ends the optional search commands and initiates the auxiliary search commands found in Table 2.1.4.

Auxiliary search commands and constraints

Auxiliary search commands are entered **only** if MORE, item 4, of the search type specification data is entered (see :numref`tab2-3`). Individual search commands are used to specify search constraints and to communicate to the search program. Searches can alter geometric dimensions (PITCH or DIMENSION Search) or alter standard composition number densities (CONCENTRATION Search).

A PITCH or DIMENSION search may require the user to specify the units that will be altered, the regions that will be altered within those units, and the faces or surfaces of those regions that will be altered. For a PITCH search, the program automatically assigns the units in the arrays to a unit cell if possible. If multiple units are contained in the array, each unit could be assigned a unit cell if the data in the unit cells match the geometry data of the units in the array. This data may be overridden in the MORE section of the search data. For a DIMENSION search, if the user wishes to tie a unit to unit cell this must be explicitly done in the MORE section of the search data. Several examples of search problems are provided in *Introduction*.

A CONCENTRATION search requires the user to specify the mixture, standard composition name, and the search constant for the component being altered. For a CONCENTRATION search, the program automatically assigns the material being changed to a unit cell. This data may be overridden in the MORE section of the search data. Several examples of search problems are provided in *Introduction*.

The data comprising the auxiliary search commands are listed in Table 7.4. All data except items 1a, 1b, and 1c are keyworded (i.e., the data are entered by specifying a keyword, followed by a value). An explanation of each individual search command follows the table.

1 Command Definition A command definition tells the code what action is to be taken. A new search command is initiated whenever an item 1a through 1c is encountered. The code will vary the geometry according to subsequent commands.

1a. ALTER CHANGE MODIFY Alter geometry regions. These words specify that modifications will be made to the geometry according to subsequent commands.

1b. MAINTAIN Maintain the thickness. The thickness of the specified geometry region(s) will be maintained when the interior regions grow or shrink (i.e., the specified region will grow or shrink in conjunction with the interior region in such a way as to maintain the original distance between the two regions). This means that the original thickness of the region is preserved. For instance, the inner radius of a pipe can be altered and the wall thickness can be preserved by applying the MAINTAIN command to the region defining the outer radius of the pipe.

1c. KEEP HOLD Keep the original specification. This command causes the specified geometry region(s) to be reset to their original input value for every search pass. Therefore they go through the entire search process unchanged.

2 PAR= Parameter number. The search parameter number is not functional. The default number is 1 and should not be overridden.

3 +CON= Maximum constraint. Enter the maximum value you wish to allow the search parameter to obtain. The maximum constraint must be larger than the minimum constraint. For a DIMENSION or PITCH search the default value of the maximum constraint is 1011. For a CONCENTRATION search the default value of the maximum constraint is as follows:

+CON= min(1/FACTOR), if any FACTOR < 0

+CON= 5*(CON), if all FACTOR > 0

Note: For a PITCH search, the maximum constraint is redefined and is calculated from the data entered for MAXPITCH. +CON should not be entered if a value was entered for MAXPITCH. If constraints, +CON= and/or CON= are not entered as data, the code computes the minimum constraint corresponding to the pins touching, and the maximum constraint is then negative five times the magnitude of the minimum constraint.

---

4 CON= Minimum constraint. Enter the minimum value you wish to allow the search parameter to obtain. The minimum constraint must be smaller than the maximum constraint but need not be a negative number. The default value of the minimum constraint for a dimension search is 1011. The default value of the minimum constraint for a pitch search is redefined to correspond to the pins in the lattice touching. For a CONCENTRATION search the default value of the minimum constraint is as follows:

CON= 5(+CON), if all FACTOR < 0

CON= max(1/FACTOR), if any FACTOR > 0

5 CELL= Unit Cell Number. This is the unit cell to which the unit or mixture will be tied. It needs to follow either the UNIT= or MIX= keyword data. Tying a unit cell to a unit or mixture ensures the unit cell data gets changed as the geometry or mixture data gets changed thus ensuring the cross sections are properly processed.

6 UNIT= Geometry unit number. This is the geometry unit to which the previously entered command definition (item 1a, 1b, or 1c) is applied. Items 7, 8, and 9 specify the region(s) within the unit and the surfaces of the region(s) to be altered.

7 REGION= First region to be altered. This is used to specify the first or only region in the unit (specified by item 6) that is to be altered according to the search command (item 1a, 1b, or 1c). The region(s) are altered according to the search constants (items 9a, 9b, 9c, and/or 9d).

8 TO Last region to be altered. This item is entered to specify the last region to be altered, starting with the region specified by REG=. For example, assume unit 3 contains eight regions and you wish to make changes to regions 4, 5, 6, 7, and 8. These regions are identified by entering the following data. UNIT=3 REG=4 TO 8.

Geometric search constants. A search constant is the proportionality factor utilized to alter a geometry region. A search constant must be entered for each surface of a region that is to be altered. A nonzero search constant will cause the region dimension for that surface to be changed. A search constant of 0.0 will cause the region dimension to remain unchanged. The default value of the search constant is 0.0.

9 ALL= Search constant for all surfaces. All of the surfaces in a region are altered simultaneously by using this search command.

9a. +X= Search constant for +X face. This parameter is used to specify the value of the search constant for the +X face of a cuboid.

9a. -X= Search constant for X face. This parameter is used to specify the value of the search constant for the X face of a cuboid.

9a. +Y= Search constant for +Y face. This parameter is used to specify the value of the search constant for the +Y face of a cuboid.

9a. -Y= Search constant for Y face. This parameter is used to specify the value of the search constant for the Y face of a cuboid.

9a. +Z= Search constant for +Z face. This parameter is used to specify the value of the search constant for the +Z face of a cuboid.

9a. -Z= Search constant for Z face. This parameter is used to specify the value of the search constant for the Z face of a cuboid.

Note: If it is desirable to change all the faces of a cuboid except the Z face by some amount (search constant of 1.0), items 9a and 9b can be used together as follows: ALL=1.0 Z=0.0. This is the same as entering +X=1.0 X=1.0 +Y=1.0 Y=1.0 +Z=1.0. If both Z faces are to remain unchanged, items 8a and 8b can be entered as: ALL=1.0 +Z=0.0 Z=0.0 or as +X=1.0 X=1.0 +Y=1.0 Y=1.0.

9b. RADIUS= Search constant for radius. This parameter is used to specify the value of the search constant for the radius of a sphere, hemisphere, cylinder, or hemicylinder.

9c. +HEIGHT= Search constant for +height. This parameter is used to specify the value of the search constant for the +height of a cylinder or hemicylinder.

9c. -HEIGHT= Search constant for height. This parameter is used to specify the value of the search constant for the height of a cylinder or hemicylinder.

9d. CHORD= Search constant for chord. This parameter is used to specify the value of the search constant for the chord of a hemisphere or hemicylinder.

10 MIX= Search constant for mixture. This parameter is the mixture number containing the standard composition that is to be changed during the search.

11 SCNAME= Search constant for the standard composition name. This parameter is the standard composition name associated with the material that is to be changed during the search. Only compositions listed in the *Standard Composition Library* section of the Standard Composition Library chapter are allowed (SECTION-REFERENCE). Standard compositions beginning with SOLN cannot be altered directly.

Note: If the standard composition name specified in the Material Information Data begins with SOLN and the Concentration Search Data specifies SCNAME=UO2(NO3)2, the amount of UO2(NO3)2 in the solution is altered but the amount of H2O and nitric acid is not altered during the search. The resulting mixture, when the search is finished, may no longer meet the criteria associated with the SOLN specification.

---

12 FACTOR= Concentration search factor used to specify the value of the search constant used in the concentration search. It is a proportionality factor used to alter the specified mixture standard composition. A search constant must be entered for each standard composition that is altered. A non-zero search constant will cause the concentration of the associated standard composition to be altered. The default value of the search constant is 1.0. A set of concentration search data consists of the mixture to be altered, the standard composition to be altered in the mixture, and the search factor. Keywords are used to enter the data. Each set of data consists of items 10, 11, and 12. The keywords used in this data may be entered using terse notation.

Table 7.4: Outline of auxiliary search commands and constraints

Entry no.	Keyword name	Type of data	Comments
GENERIC SEARCH DATA — May be used with all Search Types —			
1a	ALTER CHANGE MODIFY	Begin a new search command	These words are used to specify that modifications will be made to the geometry or concentration according to subsequent commands (entries 3 through 12 as required to specify the desired changes).
1b	MAINTAIN	Begin a new search command	The spacing (thickness) of the specified geometry regions will be maintained when the interior regions grow or shrink.
1c	KEEP HOLD	Begin a new search command	This command resets the specified geometry to the original input specifications.
2	PAR=	Parameter number	Enter the parameter number that the current command (ALTER, MAINTAIN, KEEP) applies to. Default=1 and should not be changed.
3	+CON=	Maximum constraint	Enter the maximum constraint for the current parameter. Default = +10E10.
4	CON=	Minimum constraint	Enter the minimum constraint for the current parameter. Default = 10E10.
5	CELL=	Unit Cell Associated with search data	Default values are assigned for PITCH and CONCENTRATION searches. Associated Unit Cells must be entered for a DIMENSION search if desired.
PITCH & DIMENSION SEARCH DATA — Defines Geometric Changes —			
6	UNIT=	Unit to which the current command applies	Enter the unit in which regions are to be altered.
7	REGION=	First region to be altered in the unit	Enter the first or only region in the unit that the search constants (entry 9a, b, c and/or d) apply to. Default is the first region.
8	TO	Last region to be altered in the unit	Enter the last region in the unit to which the search constants apply (entry 9a, b, c and/or d).

Table 2.1.4. Outline of auxiliary search commands and constraints (continued)			
Entry no.	**Keyword name**	**Type of data**	**Comments**
9	ALL=	Search constant for all surfaces (faces) of the region(s)	Enter a value for the search constants for the specified regions. This value will be applied to all surfaces of the region(s).
9a	+X=	Search constant for +X face of cuboid	Enter a value for the search constant for the +X face of a cuboid.
	X=	Search constant for X face of cuboid	Enter a value for the search constant for the X face of a cuboid.
	+Y=	Search constant for +Y face of cuboid	Enter a value for the search constant for the +Y face of a cuboid.
	Y=	Search constant for Y face of cuboid	Enter a value for the search constant for the Y face of a cuboid.
	+Z=	Search constant for +Z face of cuboid	Enter a value for the search constant for the +Z face of a cuboid.
	Z=	Search constant for Z face of cuboid	Enter a value for the search constant for the Z face of a cuboid.
9b	RADIUS=	Search constant for radius	Enter a value for the search constant for the radius of a sphere or a cylinder.
9c	+HEIGHT=	Search constant for +height	Enter a value for the search constant for the +height of a cylinder.
	HEIGHT=	Search constant for height	Enter a value for the search constant for the height of a cylinder.
9d	CHORD=	Search constant for chord	Enter a value for the search constant for the chord face of a hemisphere or hemicylinder.
CONCENTRATION SEARCH DATA — Defines concentration changes —			
10	MIX=	Search constant for mixture	Enter the mixture number containing the standard composition to be changed.
11	SCNAME=	Search constant for Standard Composition	Enter the standard composition name whose density is to be changed.
12	FACTOR=	Search proportionality constant	Enter the value of the search constant for the concentration search.

7.5 Example problems

This section contains example problems to demonstrate some of the options available in CSAS5 and its associated sequences. A brief problem description and the associated input data for multigroup mode of calculation are included for each problem. The same sample problems may be executed in the continuous energy mode by changing the library name from "v7-238" to "ce_v7". The sample problems can also be executed with the multigroup or continuous energy libraries based on ENDF/B-VII.1. The complete list of libraries distributed with SCALE is provided in the Nuclear Data Libraries (SECTIONREFERENCE) section of the SCALE manual. Note that sample problems 3, 7, and 8 do not run in the continuous energy mode because they use CELLMIX or DOUBLEHET cell type. See Appendix A (CSAS5App) for additional and historical examples.

7.5.1 Sample problem 1: k_{eff} calculation

The purpose of this problem is to calculate the k-effective of a system. This problem is the same as the KENO V.a sample problem 12 in Appendix B (SECTIONREFERENCE) except the cross-section library and KENO V.a mixing table are prepared by CSAS. The problem represents a critical experiment consisting of a composite array [Tho73][Tho64] of four highly-enriched (93.2%) uranium metal cylinders having a density of 18.76 g/cc and four 5.0677-L Plexiglas containers filled with uranyl nitrate solution. The uranium metal cylinders have a radius of 5.748 cm and a height of 10.765 cm. The uranyl nitrate solution has a specific gravity of 1.555 and contains 415 g of uranium per liter. The ID of the Plexiglas bottle is 19.05 cm and the inside height is 17.78 cm. The Plexiglas is 0.635 cm thick. The center-to-center spacing between the metal units is 13.18 cm in the Y direction and 13.45 cm in the Z direction. The center-to-center spacing between the solution units is 21.75 cm in the Y direction and 20.48 cm in the Z direction. The spacing between the Y-Z plane that passes through the centers of the metal units and the Y-Z plane that passes through the centers of the solution units is 17.465 cm in the X direction.

The metal units in this experiment are designated in Table II of Ref. 2 as cylinder index 11 and reflector index 1. A photograph of the experiment, Fig. 9 in Ref. 3, is given in Fig. 7.1.

```
=csas5   parm=(centrm)

s
a
m
p
l
e
p
r
o
b
l
e
m 1
s
e
t
u
p 4
a
q
u
e
o
u
s 4
m
e
t
a
l
i
n
c
s
a
s5

v7
-238
```

(continues on next page)

(continued from previous page)

```
read
 composition

u
r
a
n
i
u
m        1 0
.985 300
.  92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

s
o
l
u
t
i
o
n

m
i
x
=2

r
h
o
[
u
o2
(
n
o3
)2
]
= 415
. 92235 92
.6 92238 5
.9 92234 1
.0  92236 0
.5

m
o
l
a
r
[
h
n
o3
]
=9
.783
-3
```

(continues on next page)

(continued from previous page)

```
t
e
m
p
e
r
a
t
u
r
e
=300
  end
 solution

p
l
e
x
i
g
l
a
s
s     3 end
end
 composition
read
 param

f
l
x
=
y
e
s
f
d
n
=
y
e
s
n
u
b
=
y
e
s
end
 param
read
 geom
```

(continues on next page)

```
u
n
i
t
 1
```

(continued from previous page)

```
c
o
m
='uranyl nitrate solution in a plexiglas container'

c
y
l
i
n
d
e
r  2 1 9
.525 2
p8
.89

c
y
l
i
n
d
e
r  3 1 10
.16 2
p9
.525

c
u
b
o
i
d  0 1 4
p10
.875 2
p10
.24

u
n
i
t 2

c
o
m
='uranium metal cylinder'

c
y
l
i
n
d
e
r  1 1 5
.748 2
p5
.3825
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d  0 1 4
p6
.59 2
p6
.225

u
n
i
t 3

c
o
m
='1x2x2 array of solution units'

a
r
r
a
y 1 3
*0
.0

u
n
i
t 4

c
o
m
='1x2x2 array of metal units padded to match solution array'

a
r
r
a
y 2 3
*0
.0

r
e
p
l
i
c
a
t
e 0 1 2
*0
.0 2
*8
.57 2
*8
.03 1
```

(continues on next page)

(continued from previous page)

```
g
l
o
b
a
l
u
n
i
t 5

a
r
r
a
y 3 3
*0
.0
end
 geom
read
 array

a
r
a
=1
n
u
x
=1
n
u
y
=2
n
u
z
=2
f
i
l
l
f1 end
 fill

a
r
a
=2
n
u
x
=1
n
u
```

(continues on next page)

```
y
=2
n
u
z
=2
f
```

(continued from previous page)

```
g
b
l
=3
a
r
a
=3
n
u
x
=2
n
u
y
=1
n
u
z
=1

c
o
m
='composite array of solution and metal units'

f
i
l
l 4 3 end
 fill
end
 array
end
 data
end
```

7.5.2 Sample problem 2: optimum pitch search using detailed geometry

This problem represents an attempt to optimize the reactivity of PWR-like fuel bundles in a storage pool. The storage array is an infinite planar array of flooded fuel bundles. Each bundle consists of a 17 × 17 × 1 array of 2.35%-enriched UO_2 pins, density 9.21 g/cc, clad with Zircaloy-2. The fuel is 0.823 cm in diameter, the clad diameter is 0.9627 cm, and the length of each pin is 366 cm. Each fuel bundle is encased in a Boral sheath. There is a 1/4-in. gap flooded with water between the bundle and the sheath. The Boral sheath is 3/8 in. thick. One inch of water separates the fuel bundle sheaths in the horizontal plane, and 15 cm of water is present on the top and bottom of the array.

The KENO V.a geometry represents each fuel pin in the bundle discretely. The search should determine the optimum pitch within the fuel bundle. The gap between the bundle and the Boral remains fixed, as does the thickness of the sheath and the spacing between sheaths.

```
=csas5s

s
a
m
p
l
e
p
r
o
b
```

(continues on next page)

Fig. 7.1: Critical assembly of four solution units and four metal units.

(continued from previous page)

```
v7
-238
read
 composition

u
o2    1
.84 300
.
. 92235 2
.35 92238 97
.65 end

z
i
r
c2  2 1 end

h2
o    3 1 end

b4
c    4
d
e
n
=2
.65 0
.3517 end

a
l     4
d
e
n
=2
.65 0
.6483 end

h2
o    5 1 end
end
 composition
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
g
u
a
r
e
```

(continues on next page)

(continued from previous page)

```
end
 celldata
read
 param

n
u
b
=
y
e
s
f
a
r
=
y
e
s
g
e
n
=103
n
p
g
=500
g
a
s
=
n
o
f
d
n
=
y
e
s
end
 param
read
 geom

u
n
i
t 1

c
y
l
i
n
d
e
r  1 1
.4115 183
.0
.183
.0
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r  2 1
.48135 183
.1
-183
.1

c
u
b
o
i
d    3 1
.63755
-
.63755
.63755
-
.63755 183
.1
-183
.1

g
l
o
b
a
l
u
n
i
t 2

a
r
r
a
y     1 3
*0
.0

r
e
f
l
e
c
t
o
r 5 1 4
*0
.635  2
z  1
```

(continues on next page)

(continued from previous page)

```
r
e
f
l
e
c
t
o
r 4 1 4
*0
.9525 2
z     1

r
e
f
l
e
c
t
o
r 5 1 4
*1
.27   2
z     1

r
e
f
l
e
c
t
o
r 5 2 4
z        2
*3
.0 5
end
 geom
read
 array

a
r
a
=1
n
u
x
=17
n
u
y
=17
n
u
z
=1
i
i
l
l
```

(continues on next page)

(continued from previous page)

```
end
 array
read
 bounds

x
y
f
=
m
i
r
r
o
r
end
 bounds
read
 bias

i
d
=500 2 6
end
 bias
end
 data
read
 search

o
p
t
i
m
u
m
p
i
t
c
h
end
 search
end
```

7.5.3 Sample problem 3: optimum pitch search using homogenized geometry

This problem illustrates the use of a cell-weighted mixture to represent a PWR-like fuel bundle. The cask contains a 2 × 2 × 1 array of fuel bundles. Each fuel bundle consists of a 17 × 17 × 1 array of Zircaloy-2 clad, 2.35%-enriched UO_2 fuel pins with a density of 9.21 g/cc arranged in a square pitch. The pin diameter is 0.823 cm, and its length is 366 cm. The clad is 0.06985 cm thick, and the pitch is 1.275 cm. Each fuel bundle is contained in a 0.6625-cm-thick Boral sheath. The bundles are separated by 1 cm of water, representing a flooded cask. The square aluminum cask is 10-cm thick on all faces and is reflected by 15 cm of water.

By using CELLMIX=, a cell-weighted cross section is created to represent the fuel bundle. The KENO V.a geometry utilizes the cell-weighted mixture (500) and the overall dimensions of the fuel bundle to represent the entire fuel bundle as a single homogeneous region. The first reflector entry represents the fuel cask, and the second reflector entry represents the 15-cm reflector. Because this problem utilizes a cell-weighted mixture, which is not applicable in the continuous energy mode, the problem will end with an error message in the continuous energy mode.

```
=csas5s

s
a
m
p
l
e
p
r
o
b
l
e
m 3
s
a
m
p
l
e
s
q
u
a
r
e
f
u
e
l
c
a
s
k

v7
-238
read
 composition

u
o2    1
.84 300
. 92235 2
.35 92238 97
.65 end
```

(continues on next page)

(continued from previous page)

```
z
i
r
c2  2 1 end

h2
o    3 1 end

b4
c    4
d
e
n
=2
.65 0
.3517 end

a
l     4
d
e
n
=2
.65 0
.6483 end

h2
o    5 1 end

a
l     6 1 end
end
 composition
read
 celldata

l
a
t
t
i
c
e
c
e
l
l

s
q
u
a
r
e
p
i
t
c
h
p
i
t
c
```

(continues on next page)

(continued from previous page)

```
end
 celldata
read
 param

n
u
b
=
y
e
s
f
a
r
=
y
e
s
g
e
n
=103
n
p
g
=500
g
a
s
=
n
o
f
d
n
=
y
e
s
end
 param
read
 geom

u
n
i
t 1

c
u
b
o
i
d  500 1 4
p10
.8375 2
p183
.0
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d    4 1 4
p11
.5    2
p183
.0

c
u
b
o
i
d    5 1 4
p12
.0    2
p183
.0

g
l
o
b
a
l
u
n
i
t 2

a
r
r
a
y     1 3
*0

r
e
f
l
e
c
t
o
r 6 1 6
*10
.0 1

r
e
f
l
e
c
t
o
r 5 2 6
*3 5
```

(continues on next page)

(continued from previous page)

```
end
 geom
read
 array

a
r
a
=1
n
u
x
=2
n
u
y
=2
n
u
z
=1
f
i
l
l
f1 end
 fill
end
 array
read
 bias

i
d
=500 2 6
end
 bias
end
 data
read
 search

o
p
t
i
m
u
m
p
i
t
c
h
end
 search
end
```

7.5.4 Sample problem 4: search for a specified value of k_{eff}

Find the pitch at which a 2 × 2 × 2 array of cylinders of highly enriched (93.2%) uranium metal with a density of 18.76 g/cc are critical. Each cylinder has a radius of 5.748 cm and a height of 10.765 cm. The surface-to-surface spacing between the units is the same in all directions. The initial guess for the critical surface-to-surface spacing was 3.0 cm. The experimentally critical surface-to-surface separation for this system is 2.248 cm. The input data for this problem are given below.

```
=csas5s

s
a
m
p
l
e
p
r
o
b
l
e
m 4
c
r
i
t
i
c
a
l
p
i
t
c
h
s
e
a
r
c
h
f
o
r
c
a
s
e 2
c8
b
a
r
e

v7
-238
```

(continues on next page)

(continued from previous page)

```
read
 comp

u
r
a
n
i
u
m  1 0
.985 300
.   92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end
end
 comp
read
 parameters

 flx
=yes
 fdn
=yes
 far
=yes
 gas
=no
 rnd
=
6
5
6
6
5
1ed
2
4de
end
 parameters
read
 geometry

u
n
i
t 1

c
y
l
i
n
d
e
r 1 1 5
.748 5
.3825
=5
.3825
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d  0 1 4
p7
.248 2
p6
.8825
end
 geometry
read
 array

c
o
m
='single unit problem with 1 array is filled with unit 1'

a
r
a
=1
g
b
l
=1
n
u
x
=2
n
u
y
=2
n
u
z
=2
f
i
l
l
f1 end
 fill
end
 array
end
 data
read
 search


 critical
 pitch
```

(continues on next page)

```
 maxpitch
1
5
.
-
```

(continued from previous page)

```
a
l
t
e
r
u
n
i
t
=1
r
e
g
=2
+
z
=1
.0531
-
z
=1
.0531
end
 search
end
```

7.5.5 Sample problem 5: solution conc. search for a specified k_{eff}

Consider a large spherical tank partially filled with UO_2F_2 solution. The tank has a radius of 34.6 cm and is filled with solution to a height of 30.0 cm above the midpoint. The tank is composed of a 0.759 cm thick Al shell. The UO_2F_2 solution is composed of three standard compositions: UO2F2, HF acid, and H2O. The code combines these using a set algorithm. This may or may not produce a solution at the desired density. If the density of the solution is known it should be entered. Also, extra acid can be added to the solution by specifying a non-zero acid molarity.

A critical concentration search is performed on the solution yielding system k_{eff} = 1.0 for various densities of UO_2F_2 in the solution. In the MORE search data, MIX=1 and SCNAME=UO2F2 specify that the UO_2F_2 component of the mixture 1 solution is to be altered during the search. The code calculates the density of the solution. The initial uranium fuel density is 300 gm/liter. The maximum allowed uranium density is 600 gm/liter. The minimum allowed uranium density is 150 gm/liter.

```
=csas5s

s
a
m
p
l
e
p
r
o
b
l
e
m 5
s
o
l
n
t
a
```

(continues on next page)

(continued from previous page)

```
v7
-238
read
 composition

s
o
l
u
t
i
o
n

m
i
x
=1

r
h
o
[
u
o2
f2
]
= 300  92235 80 92238 19
.98 92234 0
.02

t
e
m
p
= 300
  end
 solution

a
l         2 1
.0 300
.0 end
end
 composition
read
 geom

g
l
o
b
a
l
u
n
i
t 1
```

(continues on next page)

(continued from previous page)

```
h
e
m
i
s
p
h
e
-
z  1 1 16
c
h
o
r
d 15
.5

s
p
h
e
r
e      0 1 16

s
p
h
e
r
e      2 1 16
.1
end
 geom
end
 data
read
 search

c
r
i
t
i
c
a
l
c
o
n
c
e
n
t
r
a
t
i
o
n
k
e
f
=1
```

(continues on next page)

(continued from previous page)

```
m
o
r
e

a
l
t
e
r
m
i
x
=1
s
c
n
a
m
e
=
u
o2
f2
f
a
c
t
o
r
=1
.0

-
c
o
n
=
-0
.5
+
c
o
n
=1
.0
end
 search
end
```

7.5.6 Sample problem 6: dimension chord search for a specified k_{eff}

Consider a large spherical tank partially filled with UO_2F_2 solution. The tank has a radius of 34.6 cm and is filled with solution to an initial height of 10.0 cm above the midpoint. The tank is composed of a 0.759 cm thick Al shell. The UO_2F_2 solution is composed of three standard compositions: UO2F2, HF acid, and H2O. The code combines these using a set algorithm. This may or may not produce a solution at the desired density. If the density of the solution is known it should be entered. Also, extra acid can be added to the solution by specifying a non-zero acid molarity.

A critical dimension search is performed on the chord length yielding system *keff* = 0.98. In the MORE search data, UNIT=1 REG=1 CHORD=1.0 specify that the chord length in region 1 of unit 1 is to be altered during the search. The constraints are set so the chord length varies from 10.0 cm to just under 34.6 cm.

```
=csas5s

s
a
m
p
l
e
p
r
o
b
l
e
m 6
s
o
l
n
t
a
n
k
-
c
r
i
t
.
d
i
m
.
s
e
a
r
c
h
o
n
c
h
o
r
d
```

(continues on next page)

(continued from previous page)

```
v7
-238
read
 comp

s
o
l
u
t
i
o
n

m
i
x
=1

r
h
o
[
u
o2
f2
]
= 300  92235 80 92238 19
.98 92234 0
.02

t
e
m
p
= 300
  end
 solution

a
l         2 1
.0 300
.0 end
end
 comp
read
 geom

g
l
o
b
a
l
u
n
i
t 1
```

(continues on next page)

(continued from previous page)

```
h
e
m
i
s
p
h
e
-
z  1 1 16
c
h
o
r
d 10
.

s
p
h
e
r
e      0 1 16

s
p
h
e
r
e      2 1 16
.1
end
 geom
end
 data
read
 search

c
r
i
t
i
c
a
l
d
i
m
e
n
s
i
o
n
k
e
f
=0
.98
```

(continues on next page)

(continued from previous page)

```
m
o
r
e

a
l
t
e
r
u
n
i
t
=1
r
e
g
=1
c
h
o
r
d
=1
.0

-
c
o
n
=
-0
.23
+
c
o
n
=0
.23
end
 search
end
```

7.5.7 Sample problem 7 two material conc. search for a specified k_{eff}

The fuel bundles in this problem represent 17 × 17 PWR fuel assemblies. The fuel pin lattice is homogenized, making a cell-weighted mixture 100. Because this problem utilizes a cell-weighted mixture, which is not applicable in the continuous energy mode, the problem will end with an error message in the continuous energy mode. The fuel pins consist of 4.35 wt % ^{235}U having a diameter of 0.823 cm, zirconium cladding having an outer diameter of 0.9627 cm, and a pitch of 1.275 cm. The fuel bundle is represented as a 10.8375 cm × 10.8375 cm × 366 cm cuboid of mixture 100 surrounded by Boral and then water. The Boral has a density of 2.61 g/cm^3 and has an initial composed of 50.0 wt % B_4C and 50.0 wt % Al. The fuel bundles are at a fixed pitch of 13.0 cm. Boral plates surrounding the X and Y sides of each fuel assembly are 0.1625 cm thick. Full density water is between the Boral plates.

A critical concentration search is performed on the Boral plates searching for a system *keff* = 0.95. The Boral plates are at a fixed density of 2.61 gm/cc. As the density of the B_4C changes, the density of the Al changes in the opposite direction maintaining a constant Boral density. There are two entries in the MORE search data. The first entry, MIX=4 SCNAME=b4c factor=1.0 specifies that the B_4C of mixture 4 is to be altered during the search. The second entry, MIX=4 SCNAME=al factor=1.0 specifies that aluminum is to be changed in the opposite direction and proportionally to B_4C during the search. Both B_4C and Al have the same initial density of 0.5 * 2.61 = 1.305 gm/cc.

```
=csas5s

s
a
m
p
l
e
p
r
o
b
l
e
m 7
f
l
u
x
t
r
a
p
b
e
t
w
e
e
n
f
u
e
l
b
u
n
d
l
e
s
-
c
r
i
t
.
c
o
n
c
```

(continues on next page)

```
.
s
r
c
h
```

(continued from previous page)

```
v7
-238
read
 composition

u
o2    1
.84 300
. 92235 4
.35 92238 95
.65 end

z
r     2 1 end

h2
o    3 1 end

a
r
b
m
b4
c  2
.61  2  0  1  0  5000 4  6000  1  4  0
.5  300
.0 end

a
l     4
d
e
n
=2
.61 0
.5 end

h2
o    5 1
.0 end
end
 composition
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
q
u
a
r
e
p
```

(continues on next page)

(continued from previous page)

```
c
l
a
d
d
=
.9627 2
c
e
l
l
m
i
x
=100  end

m
o
r
e
d
a
t
a

b
a
l
=
n
o
n
e
  end
 more
end
 celldata
read
 param

f
a
r
=
n
o
g
e
n
=203
n
p
g
=1000
end
 param
```

(continues on next page)

(continued from previous page)

```
read
 geom

g
l
o
b
a
l
u
n
i
t 1

c
u
b
o
i
d 100 1 4
p10
.8375 2
p183
.0

c
u
b
o
i
d   4 1 4
p11
.0    2
p183
.0

c
u
b
o
i
d   5 1 4
p13
.0    2
p183
.0
end
 geom
read
 bounds

x
f
c
=
m
i
r
r
o
r
y
f
c
```

(continues on next page)

(continued from previous page)

```
end
 bounds
end
 data
read
 search

c
r
i
t
i
c
a
l
c
o
n
c
e
n
t
r
a
t
i
o
n
k
e
f
=0
.95

m
o
r
e

a
l
t
e
r
m
i
x
=4
s
c
n
a
m
e
=
a
r
b
m
b4
e
f
a
c
```

(continues on next page)

(continued from previous page)

```
a
l
t
e
r
m
i
x
=4
s
c
n
a
m
e
=
a
l
f
a
c
t
o
r
=
-1
.0

-
c
o
n
=
-0
.9
+
c
o
n
=0
.99
end
 search
end
```

7.5.8 Sample problem 8: k_∞ for a pebble bed fuel

This problem demonstrates setting up a fuel pebble from a pebble bed reactor, and calculating its k∞. The pebble consists of a fuel grain of UO_2 0.025 cm in radius, coated with 0.003 cm of pyrolitic carbon, a further coat of 0.0035 cm thick silicon carbide, with a final coat of 0.004 cm thick pyrolitic carbon. 15000 grains are packed with graphite into an internal fuel sphere of 2.5 cm radius clad with a 0.5 cm thick covering of carbon and surrounded by helium. The fuel is 8.2% enriched ^{235}U. The pebbles are stacked into an infinite square pitched array with a pitch of 6 cm.

This problem uses DOUBLEHET cell type, which is applicable only in the multigroup mode of KENO calculations. Therefore, the continuous energy version of this problem will end with an error message.

```
=csas5              parm=(centrm)

i
n
f
i
n
i
t
e
a
r
r
a
y
o
f
p
e
b
b
l
e
s
o
n
a
s
q
u
a
r
e
p
i
t
c
h

v7
-238
read
 composition
' fuel kernel

u
-238  1 0 2
.12877
e
-2 293
.9end
```

(continues on next page)

(continued from previous page)

```
u
-235  1 0 1
.92585
e
-3 293
.6 end

o      1 0 4
.64272
e
-2 293
.6 end
' inner pyro carbon

c      3 0 9
.52621
e
-2 293
.6 end
' silicon carbide

c      4 0 4
.77240
e
-2 293
.6 end

s
i     4 0 4
.77240
e
-2 293
.6 end
' outer pyro carbon

c      5 0 9
.52621
e
-2 293
.6 end
' graphite matrix

c      6 0 8
.77414
e
-2 293
.6 end
' carbon pebble outer coating

c      7 0 8
.77414
e
-2 293
.6 end

h
e
-3    8 0 3
.71220
e
-11 293
.6 end
```

(continues on next page)

(continued from previous page)

```
h
e
-4    8 0 2
.65156
e
-5 293
.6 end
end
 composition
read
 celldata

d
o
u
b
l
e
h
e
t
r
i
g
h
t
_
b
d
y
=
w
h
i
t
e
f
u
e
l
m
i
x
=10 end

g
f
r
=0
.025  1
c
o
a
t
t
=0
.004 3
c
o
a
t
t
=0
.0025 4
```

(continues on next page)

(continued from previous page)

```
m
a
t
r
i
x
=6
n
u
m
p
a
r
=15000 end
 grain

p
e
b
b
l
e
s
p
h
s
q
u
a
r
e
p
r
i
g
h
t
_
b
d
y
=
w
h
i
t
e
h
p
i
t
c
h
=3
.0 8
f
u
e
l
r
=2
.5
c
```

(continues on next page)

(continued from previous page)

```
c
e
n
t
r
m
d
a
t
a

i
x
p
r
t
=1
i
s
n
=8
n
p
r
t
=2
  end
 centrm
end
 celldata
read
 param

g
e
n
=210
n
p
g
=1000
end
 param
read
 bounds

a
l
l
=
m
i
r
r
o
r
```

(continues on next page)

(continued from previous page)

```
end
 bounds
read
 geom

g
l
o
b
a
l
u
n
i
t 1

s
p
h
e
r
e   10 1 2
.5

s
p
h
e
r
e    7 1 3
.0

c
u
b
o
i
d    8 1 6
p3
.0
end
 geom
end
 data
end
```

7.6 Warning and error messages

CSAS5 contains two types of warning and error messages. Warning messages appear when a possible error is encountered. It is the responsibility of the user to verify whether the data are correct when a warning message is encountered. The functional modules activated by CSAS5 sequences will be executed if no error messages are generated and a warning message has been generated.

When an error is recognized, an error message is written and an error flag is set so the functional modules will not be activated. The code stops immediately if the error is too severe to allow continuation of input. However, it will continue to read and check the data if it is able. When the data reading is completed, execution is terminated if an error flag was set when the data were being processed. If the error flag has not been set, execution continues. When error messages are present in the output, the user should focus on the first error message, because subsequent messages may have been caused by the error that generated the first message.

The following messages originate in the part of CSAS5 that reads, checks, and prepares data for KENO V.a and the search module MODIFY.

CS-10 * ERROR *** CONCENTRATION SEARCH MATERIAL WAS NOT SPECIFIED IN THE STANDARD COMPOSI**
This self-explanatory message from subroutine CNCN indicates that the indicated material is not in the standard composition data. Recheck the standard composition data and the search data, correct the input, and resubmit the problem.

CS-11 * ERROR *** CONCENTRATION SEARCH DATA HAS BEEN DESTROYED. I= _____ ICMND= _____ IPNUM=**
This message from subroutine CNCSRH indicates that the search data could not be read properly. This usually indicates either: search data that is required for the specified search type is missing or search data inappropriate for the specified search type is present. Recheck the search data, correct the input, and resubmit the problem.

CS-16 ***WARNING* READ FLAG NOT FOUND. ASSUME KENO V PARAMETER DATA FOLLOWS.**
This message from subroutine CPARAM indicates that the word READ is not the first word of KENO V.a data following the Material Information Processor input data. If parameter data is to be entered, the code expects the words READ PARAMETERS to precede the parameter input data. If the word READ is not the first word, the code assumes the data are parameter input data.

CS-21 A UNIT NUMBER WAS ENTERED FOR THE CROSS-SECTION LIBRARY. (LIB= IN PARAMETER DATA.) THE D
This message is from subroutine CPARAM. It indicates that a value has been entered for the cross-section library in the KENO V.a parameter data. The cross-section library created by the analytical sequence should be used. MAKE CERTAIN THAT THE CORRECT CROSS SECTIONS ARE BEING USED.

CS-50 * ERROR *** SEARCH COMMAND NUMBER _____ IS UNABLE TO PERFORM A PITCH SEARCH BECAUSE**
This message from subroutine PCHSRH indicates that the specified search command is not valid for the specified region. An ARRAY or CORE region cannot be altered; nor can a REPLICATE or REFLECTOR region immediately following an ARRAY or CORE region.

CS-55 * ERRORS WERE ENCOUNTERED IN PROCESSING THE CSAS-KENO5 DATA. EXECUTION IS IMPOSSIBLE**
This message from subroutine SASSY is printed if errors were found in the KENO V.a input data for CSAS5. If a search is being made, data reading will continue until all the data have been entered or a fatal error terminates the data reading. When the data reading and checking have been completed, the problem will terminate without executing. Check the printout to locate the errors responsible for this message.

CS-62 * ERROR *** MIXTURE _____ IN THE GEOMETRY WAS NOT CREATED IN THE STANDARD COMPOSITIO**
This message from subroutine MIXCHK indicates that a mixture specified in the KENO V.a geometry was not created in the standard composition data.

CS-68 * ERROR *** AN INPUT DATA ERROR HAS BEEN ENCOUNTERED IN THE _____ DATA ENTERED FOR THE**
This message from the main program, CSAS5, is printed if the subroutine library routine LRDERR returns a value of "TRUE," indicating that a reading error has been encountered in the "KENO PARAMETER" data or the CSAS5 "SEARCH" data. The appropriate data type is printed in the message. Locate the unnumbered

message stating "*** **ERROR IN INPUT. CARD IMAGE PRINTED ON NEXT LINE** ***." Correct the data and resubmit the problem.

CS-69 ***ERROR* MIXTURE _____ IS AN INAPPROPRIATE MIXTURE NUMBER FOR USE IN THE KENO GEOME**
This message from subroutine CMXCHK indicates that a mixture that is a component of a cell-weighted mixture has been used in the KENO V.a geometry data.

CS-70 *** ERROR ***** SEARCH OR OPTIMIZATION DATA MUST BE ENTERED FOR CSAS5. NO SEARCH DATA V**
This message from subroutine RDOPT is self-explanatory. If the user does not desire to run a search, another sequence such as CSAS5 should be chosen.

CS-71 * ERROR *** _____ IS NOT A VALID SEARCH TYPE.** This message is from subroutine RDOPT. The allowed search types include PITCH, DIMENSION, and CONCENTRATION. The first four characters of the search data after the words READ SEARCH must be PIT, PITC, DIM, DIME, DMSN, CON, or CONC. The data may be misspelled or out of order.

CS-72 * ERROR *** THE SEARCH TYPE IS INVALID. I= _____.** This message is from subroutine RDOPT. The numerical index, I, should be 1 for an optimum pitch search, 2 for a dimension search, and 3 for a concentration search. If it is none of these, the search type has been incorrectly specified or a code error has been introduced.

CS-73 *** AN END OF FILE WAS ENCOUNTERED BEFORE ALL THE SEARCH DATA WAS READ.**
This self-explanatory message is from subroutine RDOPT. Check the input data to be sure nothing was omitted or misspelled.

CS-74 *** AN END SEARCH FLAG WAS READ BEFORE ALL THE SEARCH DATA WAS READ.** This self-explanatory message is from subroutine RDOPT. Check the input data for omissions and correct order.

CS-75 * ERROR *** READ SEARCH FLAG WAS NOT FOUND. _____ WAS READ INSTEAD.** This self-explanatory message is from subroutine RDOPT. READ SEARCH was expected but was not found. Check the input data for omissions and correct order.

CS-76 * ERROR *** END SEARCH FLAG WAS NOT FOUND. _____ WAS READ INSTEAD.** This self-explanatory message from subroutine RDOPT indicates that an end of file was encountered when looking for READ SEARCH. Check the input data for omissions, correct order, and spelling.

CS-77 * ERROR *** AN END OF FILE WAS FOUND WHEN THE READ SEARCH FLAG WAS EXPECTED.**
This self-explanatory message is from subroutine RDOPT. Check the input data for omissions, correct order, and spelling.

CS-78 * ERROR *** _____ IS NOT A VALID SEARCH TYPE.** This message is from subroutines SRCHTYP. It indicates that an invalid search type was read. The valid search names include PITCH, CONCENTRATION, and DIMENSION. Either the data was entered improperly or a code error has been introduced. A STOP 215 is executed when this message is printed.

CS-80 * ERROR *** SEARCH DATA HAS BEEN DESTROYED. I= _____ ICMND= _____ IPNUM= _____ II= _____ I**
This message from subroutines DIMSRH indicates that the search data cannot be interpreted. This usually indicates either: search data that is required for the specified search type is missing or search data inappropriate for the specified search type is present. Recheck the search data, correct the input, and resubmit the problem.

CS-82 * AN ERROR WAS ENCOUNTERED IN ONE OF THE FUNCTIONAL MODULES.** This message from CSAS5 or MODIFY indicates that an error was encountered during execution of one of the functional modules such as CRAWDAD, BONAMI, CENTRM, PMC, XSDRNPM, or KENO V.a. Check the printout to locate and correct the error.

CS-83 *** NO FEASIBLE SOLUTION WAS FOUND IN THE SEARCH PACKAGE. EXECUTION IS TERMINATED.**
This message comes from the MODIFY search package, and indicates that it is unable to find a solution to the problem as presented. This usually occurs when a solution is not within the range specified. For this case the user must decide what to change to improve the possibility of a solution. Fairly rarely, for an optimum problem, there may be 2 maximums within the range specified, and the package has found the wrong one. For this case,

the user would tighten the range to be searched to eliminate the unwanted peak. The package uses least mean square fitted cubic polynomials to make guesses as to where a solution is. If the Keffectives have too much variance, the polynomials may not be a good representation of the actual behavior of the system. For this case the user could rerun the problem using more histories per pass to reduce the variance.

CS-85 * ERROR *** ALL OF THE ROOTS FOR K=_____ LIE OUTSIDE THE PARAMETER CONSTRAINTS**
This message from MODIFY indicates that the polynomial fit to the Keffectives already calculated only has solutions for the Keffective asked for outside the parameter constraints specified. Keffectives with large variances can lead to polynomials which fit the actual behavior of a system poorly. The user could rerun the case with more histories to reduce the variance, if this is the problem. If the variance is not the problem, then extending the parameter range, or making some other change to the problem definition to change the Keffective range will be necessary.

CS-89 * ERROR *** _____ IS AN INVALID DIMENSION SEARCH COMMAND.** This message from subroutine DMSN indicates that the dimension search data are out of order, a search command is spelled incorrectly, or the search data are specified incorrectly.

CS-90 * ERROR *** _____ IS AN INVALID SEARCH PARAMETER.** This message printed from subroutines CNCTYP, DIMTYP, and PCHTYP indicates that a parameter entered in the search type specification data is not valid. The data could be misspelled or out of order. Omission of the keyword MORE before entering the individual search commands can cause this error.

CS-91 * ERROR *** _____ IS AN INVALID CONCENTRATION SEARCH COMMAND.** This message from subroutine CNCN is caused by a misspelled or illegal search command when attempting to do a concentration search.

CS-94 * ERROR *** REG= _____ IS AN INVALID SEARCH DATA ENTRY. THE REGION NUMBER MUST BE GREAT**
This message from subroutine DMSN indicates that the region to be altered is incorrectly specified. For example, if the unit being altered contains five geometry regions, the value specified for REG= can be as small as 1 and as large as 5.

CS-95 * ERROR *** AN ERROR WAS ENCOUNTERED IN THE SEARCH DATA. THE LAST REGION NUMBER MUST**
This message from subroutine DMSN indicates that the search data specified an invalid region number for the final region to be altered. Check the printed data and correct as appropriate.

CS-96 * ERROR *** AN ERROR WAS ENCOUNTERED IN THE SEARCH DATA. THE REGION NUMBERS MUST BE**
This message from subroutine DMSN indicates that one of the specified region numbers is incorrect. Check the printed data and correct as appropriate.

CS-97 * ERROR *** NO VALID SEARCH COMMANDS WERE FOUND IN THE DATA.** This message is accompanied by a STOP 235 and is printed from subroutines PCHSRH, CNCSRH, and DIMSRH. A common cause of this error is the omission of the MORE command before the individual search commands are entered.

CS-99 * ERROR *** THIS PROBLEM WILL NOT BE RUN BECAUSE PARM=CHECK WAS ENTERED IN THE ANALY**
This message from subroutine CSAS5 indicates that the problem data were read and checked and no errors were found. To execute the problem, remove the PARM=CHECK or PARM=CHK from the analytical sequence indicator data entry.

CS-100 * ERROR *** THIS PROBLEM WILL NOT BE RUN BECAUSE ERRORS WERE ENCOUNTERED IN THE INPU**
This message from subroutine CSAS5 is self-explanatory. Examine the printout to locate the error or errors in the input data. Correct them and resubmit the problem.

CS-101 * ERROR *** THE CONSTRAINTS ARE NOT VALID FOR PARAMETER SET. CON= _____ +CON= _____**
This message is printed from either subroutine CNCN or DMSN if the parameter set is invalid. For a parameter set to be valid, CON must be less than 0.0 and +CON must be greater than 0.0. They can be explicitly set or calculated using default or provided data.

CS-102 * ERROR *** THE UNIT CELL SPECIFICATION FOR UNIT _____ IS OUT OF BOUNDS. CELL NUMBER ___**
This self-explanatory message from subroutine DMSN indicates that the unit cell specified is not between 1

and the number of unit cells present in the problem. Recheck the unit cell number specified in the search data, correct the input, and resubmit the problem.

CS-103 * ERROR *** THE UNIT CELL SPECIFICATION FOR MIXTURE _____ IS OUT OF BOUNDS. CELL NUMBE**

This self-explanatory message from subroutine CNCN indicates that the unit cell specified for the indicated mixture is not between 1 and the number of unit cells present in the problem. Recheck the unit cell number specified in the search data, correct the input, and resubmit the problem.

CHAPTER

EIGHT

ADDITIONAL EXAMPLE APPLICATIONS OF CSAS5

Several example uses of CSAS5 are shown in this section for a variety of applications. Note that many of these examples have been provided since the earliest versions of the CSAS sequences and output data shown may not represent the most current version.

8.1 Typical search

EXAMPLE 1. CSAS5S — Determine the optimum pitch for an array of Example 4 fuel assemblies

Consider a 4 × 4 × 1 array of fuel assemblies in a square aluminum cask. Each assembly consists of a 17 × 17 × 1 array of zirconium-clad, 2.35%-enriched UO_2 fuel pins in a square pitched array. The UO_2 has a density of 9.21 g/cc. The pin diameter is 0.8 cm and is 366 cm long. The clad is 0.07 cm thick, and the pitch is 1.3 cm. Each fuel bundle is contained in a 0.65-cm-thick Boral sheath. The bundles are separated by an edge-to-edge spacing of 1 cm. The array of bundles is centered in a 10-cm-thick aluminum cask whose inside dimensions are 0.5 cm beyond the outer edges of the fuel bundles. Search for the assembly spacing that yields the maximum value of k_{eff}. Because the spacing between the assemblies is to be altered, the last region of unit 2 will be altered. In order to do this, the fuel assembly shroud cannot be defined as a replicate, because the code does not know the size of the array until later. In order to perform a pitch or dimension search, the code calculates the distance between the outermost region of the unit and the region interior to it. Therefore, the fuel assembly gap must be defined as a cuboid, and the water gap between assemblies can be entered as either a cuboid or a replicate. This search has been defined as an optimum dimension search. The input data for this problem follow.

```
=CSAS5S

S
A
M
P
L
E
F
U
E
L
C
A
S
K
E
X
A
M
P
L
E
```

(continues on next page)

(continued from previous page)

```
V7
-238

R
E
A
D
C
O
M
P

U
O2 1
D
E
N
=9
.21 1
.0 293
.  92235 2
.35 92238 97
.65
E
N
D

Z
R 2 1
E
N
D

H2
O 3 1
E
N
D

B4
C 4 0
.367
E
N
D

A
L 4 0
.636
E
N
D

A
L 5 1
E
N
D
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
Q
U
A
R
E
P
I
T
C
H
P
I
T
C
H
=1
.3 3
F
U
E
L
D
=0
.8 1
C
L
A
D
D
=0
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
P
A
R
A
M
T
M
E
=6
.0
N
U
B
=
Y
E
S
F
A
R
=
Y
E
S
G
E
N
=103

E
N
D
P
A
R
A
M

R
E
A
D
G
E
O
M
U
```

(continues on next page)

(continued from previous page)

```
C
Y
L
I
N
D
E
R 1 1 0
.4 2
P183
.0
C
Y
L
I
N
D
E
R 2 1 0
.47 2
P183
.07

C
U
B
O
I
D 3 1 4
P0
.65 2
P183
.07

U
N
I
T 2

C
O
M
='FUEL ASSEMBLY'

A
R
R
A
Y 1 2
R
-11
.05
-183
.07
C
U
B
O
I
D 4 1 4
P11
.7 2
P183
```

(continues on next page)

(continued from previous page)

```
R
E
P
L
I
C
A
T
E 3 1 6
*0
.5 1

G
L
O
B
A
L
U
N
I
T 3

C
O
M
='FUEL CASK CONTAINING 4X4 ARRAY OF ASSEMBLIES'

A
R
R
A
Y 2 2
R
-48
.8
-184
.22

R
E
P
L
I
C
A
T
E 5 1 6
R10
.0 1

E
N
D
G
E
O
M
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y
A
R
A
=1
N
U
X
=17
N
U
Y
=17
N
U
Z
=1
F
I
L
L
F1
E
N
D
F
I
L
L

A
R
A
=2
N
U
X
=4
N
U
Y
=4
N
U
Z
=1
F
I
L
L
F2
E
N
D
F
```

(continues on next page)

(continued from previous page)

```
E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A

R
E
A
D
S
E
A
R
C
H
O
P
T
I
M
U
M
D
I
M
E
N
S
I
O
N
M
O
R
E

A
L
T
E
R
U
N
I
T
=2
R
E
G
=3
+
```

(continues on next page)

(continued from previous page)

```
+
C
O
N
=0
.204918
-
C
O
N
=
-0
.0409836

E
N
D
S
E
A
R
C
H

E
N
D
```

An alternative method of entering the search data for this problem is to define the search as an optimum pitch search and require that the spacing of the fuel pin cells remain unchanged. Because a pitch search is always conducted at the lowest array level, in this case the spacing between the pins in the fuel assembly (the outer region of unit 1), it is necessary to countermand the automatic alteration of the outer region of unit 1 by entering the KEEP command. Search constants must be entered for the X and Y faces to instruct the code to KEEP those dimensions unchanged. It is easier to use the keyword ALL, which applies the KEEP command to all of the faces since the optimum pitch search would have changed only the X and Y faces leaving the Z faces unchanged. The ALTER command must then be entered to instruct the search to alter the spacing between the fuel assemblies (region 3 of unit 2). Only the X and Y dimensions are to be altered; so the search constants are entered individually for those dimensions. It is acceptable to enter ALL=1 +Z=0 Z=0 rather than +X=1 X=1 +Y=1 Y=1. It is not necessary to enter the constraints for an optimum pitch search (+CON= and CON=). They were entered in this case to ensure that the alternative data more nearly duplicate the optimum dimension search data from the previous example. These alternative search data are:

```
R
E
A
D
S
E
A
R
C
H
O
P
T
I
M
U
M
P
I
T
```

(continues on next page)

(continued from previous page)

```
K
E
E
P
U
N
I
T
=1
R
E
G
=3
A
L
L
=1

A
L
T
E
R
U
N
I
T
=2
R
E
G
=3
+
X
=1

X
=1
+
Y
=1

Y
=1
E
N
D
S
E
A
R
C
H
```

8.2 Auxiliary search commands

Auxiliary search commands are entered ONLY if the word MORE was entered in the search type specification data. These data are used to define the method the search will use to alter the pitch, geometry or concentration data and to set the constraints for the parameter search. The auxiliary search commands consist of (1) INDIVIDUAL SEARCH COMMANDS and (2) SEARCH PARAMETER CONSTRAINTS.

EXAMPLE 1

Consider an example in which region 2 of unit 1 is a cuboid and all of the dimensions of the cuboid are to be altered. The search data could be entered as:

```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=2
A
L
L
=1
.0
```

or

```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=2
+
X
=1
.0

X
=1
.0
+
Y
=1
.0

Y
=1
```

(continues on next page)

(continued from previous page)

Because all of the search constants are nonzero, all of the dimensions will be changed. Because the search constants are identical, the original relationship between the dimensions will be preserved as they are altered.

For example, if region 2 of unit 1 is a cylinder and if all the dimensions of the cylinder are to be altered, and if unit 1 is tied to unit cell 1 the search data could be entered as:

```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=2
A
L
L
=1
.0
C
E
L
L
=1
```

or

```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=2
R
A
D
I
U
S
=1
.0
+
H
=1
.0
?
H
```

(continues on next page)

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Because all of the search constants are nonzero, all of the dimensions will be changed. Because the search constants are identical, the original relationship between the dimensions will be preserved as they are altered. If the original height-to-diameter ratio is 1.5, that ratio will be preserved throughout the search only if the search constants for the radius and + and height are identical.

Search constants can be entered sequentially with each new entry overriding only identical previous entries. For example, if region 2 of unit 1 is a cuboid and if all of the dimensions except the Z dimension are to be altered, the search data could be entered as:

```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=2
+
X
=1
.0

X
=1
.0
+
Y
=1
.0

Y
=1
.0
+
Z
=1
.0
```

or

```
A
L
T
E
R
U
N
I
T
=1
E
G
=2
A
```

(continues on next page)

(continued from previous page)

In the second example, all of the search constants corresponding to the cuboid's dimensions are set to 1.0 by using the ALL= command. This includes the Z dimension. To reset the search constant for the Z dimension to zero, Z=0.0 is added following the ALL=1.0 command. If the search commands are reversed, Z=0.0 ALL=1.0, the Z dimension will also be altered because the Z portion of the ALL= command will override the previously entered Z=0.0 command.

EXAMPLE 2

A search command must be entered for each unit and region specification. Consider a problem having units 1, 2, and 3. Unit 1 consists of three concentric spheres in a cuboid. Unit 2 consists of a single sphere in a cuboid, and unit 3 contains three concentric cuboids. A search is to be made that changes the inner sphere and outer cuboid of unit 1, and the sphere and cuboid of unit 2, and the exterior cuboid of unit 3. The thicknesses of the outer spheres of unit 1 are to be maintained, and the two inner cuboids of unit 3 are to remain unchanged. The search data for this problem can be entered as follows:

```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=1
A
L
L
=1
.0

A
L
T
E
R
U
N
I
T
=1
R
E
G
=4
A
L
L
=1
.0
M
A
I
N
```

(continues on next page)


```
A
I
N
U
```

(continued from previous page)

8.3 Search constraints for dimension or pitch searches

SEARCH PARAMETER CONSTRAINTS set the parameter limits for the search. The minimum constraint is the minimum value of the parameter allowed in the search. The maximum constraint is the maximum value of the parameter allowed in the search. The initial geometry configuration corresponds to a parameter value of 0.0. A physical limit occurs when the value of the parameter causes geometry intersections. Constraints should be entered for a DIMENSION search. Only one set of constraints (i.e., min and max) are allowed per problem. These constraints apply to all the dimensions that are being altered.

For a DIMENSION search, the constraints are given by (8.1) and (8.2)

$$C_{min} = ((D_{min}/D_i) - 1.0)/SC, \tag{8.1}$$

$$C_{max} = ((D_{min}/D_i) - 1.0)/SC, \tag{8.2}$$

Where

C_{min} is the minimum constraint for the search

C_{max} is the maximum constraint for the search

D_{min} is the minimum allowed dimension for the search [For a chord, D_{min} = (Radius:sub:*min* + $Chord_{min}$)/ 2 Radius] min

D_{max} is the maximum allowed dimension for the search [For a chord, D_{max} = (Radius:sub:*max* + $Chord_{max}$)/ 2 $Radius_{max}$]

D_i is the initial dimension [For a chord, D_i = (Radius:sub:*initial* + $Chord_{initial}$)/2 $Radius_{initial}$]

SC is the search constant for that dimension (i.e., +X, X, RADIUS, etc.)

For example, the initial radius of a sphere is 6 cm, and a search is to be conducted to determine the radius at which the sphere is critical. The minimum radius the user wishes to allow is 3 cm, and the maximum radius to be allowed is 9 cm. A nonzero search constant must be entered to cause the radius to be changed. A search constant of 1.0, will be used for the radius (RADIUS=1.0). The constraints calculated from (8.1) and (8.2) are:

C_{min} = ((3.0/6.0)1.0)/1.0 = 0.5

C_{max} = ((9.0/6.0)1.0)/1.0 = 0.5

The constraints would be entered in the problem by entering the following data:

```
-
C
O
N
=
-0
.5
+
C
O
N
=0
.5
```

(continues on next page)

(continued from previous page)

For a PITCH search, the minimum constraint defines the limit for shrinking the system, and the maximum constraint defines the limit for expanding the system:

$$C_{min} - \text{MAX}\,[D_+, D_] \text{ for shrinking ,} \quad \text{i = number of faces, i=1}$$

$$C_{max} - \text{MIN}\,[D_+, D_] \text{ for expanding ,} \quad \text{i = number of faces, i=1}$$

where

C_{min} is the minimum constraint,

C_{max} is the maximum constraint,

D_+ are face constraints for the positive dimensions,

D are face constraints for the negative dimensions.

Face constraints must be calculated for each face using (8.3) and (8.4) :

$$D_+ = \frac{(X_{d+} - X_{i+})(SC_+ \times \text{del}_+\text{SC_} \times \text{del_})}{(X_{i+} - X_{i-})(\text{SC}_+\text{**2} \times \text{del_})} \tag{8.3}$$

$$D_ = \frac{(X_{d-} - X_{i-})(SC_+ \times \text{del}_+\text{SC_} \times \text{del_})}{(X_{i+} - X_{i-})(\text{SC}_+\text{**2} \times \text{del_})} \tag{8.4}$$

where

X_{d+} is the desired limit of the positive dimension of the spacing cuboid in that direction (positive dimension of X, Y, or Z, whichever dimension is under consideration)

X_{i+} is the initial positive dimension of the spacing cuboid in that direction (positive dimension of X, Y, or Z, whichever dimension is under consideration)

X_d is the desired limit of the negative dimension of the spacing cuboid in that direction (negative dimension of X, Y, or Z, whichever dimension is under consideration)

X_i is the initial negative dimension of the spacing cuboid in that direction (negative dimension of X, Y, or Z, whichever dimension is under consideration)

SC_+ is the search constant for the positive dimension of the spacing cuboid in that direction (positive dimension of X, Y, or Z, whichever dimension is under consideration)

SC is the search constant for the negative dimension of the spacing cuboid in that direction (negative dimension of X, Y, or Z, whichever dimension is under consideration)

Note: Using a search constant of 1.0 simplifies the determination of C_{max} and C_{min} when the dimensions are to change proportionately.

del_+ is the initial distance from the spacing cuboid to the closest interior region in the positive direction (positive dimension of X, Y, or Z, whichever dimension is under consideration)

del is the initial distance from the spacing cuboid to the closest interior region in the negative direction (negative dimension of X, Y, or Z, whichever dimension is under consideration)

The search parameter constraints are entered using the following keywords:

CON=pp is used to set the minimum constraint for the current parameter. The value of pp is defaulted to 10E10 for a dimension search. The value of pp is defaulted to a value that allows geometry regions to touch for a pitch search unless a value was entered for MINPITCH, in which case the parameter corresponding to that pitch is calculated and used.

+CON=rr is used to set the maximum constraint for the current parameter. The value of rr is defaulted to +10E10 for a dimension search and to 5 × pp for a pitch search.

Note: A search will reset a constraint (entered using the keyword +CON= or CON=) that falls outside the default range to the default value. If a PITCH search is specified and if a value has been entered for MAXPITCH and/or MINPITCH, values should not be entered for the constraints. If values are entered for +CON= and/or CON= for a PITCH search and if MAXPITCH and/or MINPITCH were specified in the optional search parameters, the maximum and minimum constraints will be set to the values corresponding to MAXPITCH and MINPITCH, even though the value of MINPITCH may result in an intersection.

8.3.1 Individual concentration search commands

An INDIVIDUAL SEARCH COMMAND for a concentration search consists of (1) a command definition, (2) the mixture number of the mixture to be altered, (3) the name of the standard composition to be altered, (4) a search constant, and (5) a unit cell containing the mixture. A series of individual search commands can be entered to govern the search process. A new search command is initiated whenever a command definition, item (1) above, is encountered.

The COMMAND DEFINITION defines the action to be taken for the specified mixture and standard composition component. ALTER, CHANGE, or MODIFY are used to cause the concentration (number densities) of the specified standard composition in the specified mixture to be modified.

ALTER CHANGE MODIFY The commands to the left are command definitions, item (1) above. These commands instruct the code to modify the specified concentration data.

The MIXTURE NUMBER, item (2) above, defines the mixture that contains the standard composition whose concentration is to be varied during the search. The keyword **MIX=** is entered, followed by the mixture number, nn.

MIX=nn is used to define the mixture number associated with the component that is to be changed. The keyword MIX= is entered, followed by the mixture number, nn. There is no default value of nn.

The STANDARD COMPOSITION NAME, item (3) above, defines the standard composition whose concentration will be changed in the defined mixture. Only standard compositions listed in the Standard Composition Library chapter can be entered.

SCNAME=mm is used to specify the standard composition name of the component that is to be altered. The keyword SCNAME= is entered, followed by the mixture number, mm. There is no default value for mm.

Note: If the standard composition component name specified in the Material Information Data (item 1 of the Standard Composition Specification Data) is a solution, for example, SOLNUO2(NO3)2, and the Concentration Search Data specifies SCNAME=UO2(NO3)2, the amount of UO2(NO3)2 in the solution will be altered, but the amount of water and nitric acid will not be changed. Thus, the resultant mixture may no longer meet the criteria associated with the SOLN specification.

The SEARCH CONSTANT for a concentration search, item (4) above, is a proportional factor that applies to the standard composition being altered. The keyword FACTOR= followed by a proportionality search constant is used to specify the search constant for a concentration search.

FACTOR=pc is used to specify the search constant. The keyword FACTOR= is entered, followed by the value of the search constant or proportionality factor, pc.

The UNIT CELL NUMBER, item (5) above, defines the unit cell containing the mixture to be varied during the search. The keyword **CELL=** is entered, followed by the unit cell number, mm.

CELL=mm is used to link mixture nn to unit cell mm. The keyword CELL= is entered, followed by the unit cell number, mm. The code defaults the cell number to the unit cell containing the mixture specified using MIX=.

ENTERING AUXILIARY SEARCH COMMANDS IN THE CONCENTRATION SEARCH DATA

EXAMPLE 1

Consider an example in which the density of water is to be varied and is contained in unit cell 2. Full density water, mixture 1, was specified in the standard composition specification data as: H2O 1 END The auxiliary search data could be entered as follows:

```
A
L
T
E
R
M
I
X
=1
S
C
N
A
M
E
=
H2
O
F
A
C
T
O
R
=1
.0
C
E
L
L
=2


o
r


A
L
T
E
R
M
I
X
=1
S
```

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(continued from previous page)

```
o
r


A
L
T
E
R
M
=1
S
=
H2
O
F
=1
.0
C
=2
```

Note that terse input allows truncation of the keywords.

EXAMPLE 2

Consider an example in which the density of UO_2F_2, is to be varied in mixture 2 contained in unit cell 4, a uranyl fluoride solution. The uranyl fluoride solution was specified as:

```
S
O
L
N
U
O2
F2   2   300   0   1   293   92235   5   92238   95
E
N
D
```

The auxiliary search data could be entered as follows:

```
A
L
T
E
R
M
I
X
=2
S
C
N
A
```

(continues on next page)

```
M
E
S
U
O2
F2
F
```

(continued from previous page)

```
o
r


A
L
T
E
R
M
=2
S
=
U
O2
F2
F
=1
C
=4
```

The terse input option allows truncation of the keywords.

8.4 Search constraints for concentration searches

A SEARCH PARAMETER CONSTRAINT for concentration searches sets the parameter limits for the search. The minimum constraint is the minimum value of the parameter allowed in the search. The maximum constraint is the maximum value of the parameter allowed in the search. The initial concentration corresponds to a parameter value of 0.0. A physical limit occurs when the value of the parameter causes the density of the specified standard composition to become negative. The search can produce an unrealistically high density. Users should manually eliminate those results or set constraints to avoid them. Only one set of constraints (i.e., min and max) are allowed per problem. These constraints apply to all the standard compositions that are being altered.

For a CONCENTRATION search, the constraints are given by (8.5) and (8.6). The maximum constraint must be larger than the minimum constraint.

$$C_{min} = \frac{((\frac{D_{min}}{D_i}) - 1)}{\text{FACTOR}}, \tag{8.5}$$

$$C_{max} = \frac{((\frac{D_{max}}{D_i}) - 1)}{\text{FACTOR}}, \tag{8.6}$$

where

C_{min} is the minimum constraint for the search,

C_{max} is the maximum constraint for the search,

D_{min} is the minimum allowed density for the specified standard composition,

D_{max} is the maximum allowed density for the specified standard composition,

D_i is the initial density of the specified standard composition,

FACTOR is the search constant for the standard composition that is being varied.

Default search constraints are calculated if +CON and CON are not entered. The default concentration search constraints are calculated as follows:

$$+\text{CON} = \begin{Bmatrix} \min(\frac{1}{FACTOR}), \text{if any FACTOR} < 0 \\ \text{-S} \times (\text{-CON}), \text{if all FACTOR} > 0 \end{Bmatrix}$$

$$-\text{CON} = \begin{Bmatrix} \text{-S}(+\text{CON}), \text{if all FACTOR} < 0 \\ \max(\frac{-1}{FACTOR}), \text{if any FACTOR} > 0 \end{Bmatrix}$$

8.5 Search considerations

DIMENSION, PITCH, and CONCENTRATION searches can be performed using CSAS5S. A DIMENSION search alters only those regions specified in the search data. A PITCH search alters the center-to-center spacing of units in an array and any other dimensions specified in the auxiliary data. A CONCENTRATION search alters the density of the standard compositions in the mixtures specified.

By default a pitch search is performed at the lowest array level and changes the spacing in either the X dimension for a slab, the X and Y dimensions for an array of cylinders, or the X, Y and Z dimensions for an array of spheres. For example, if an array of fuel assemblies is described in the geometry, the lowest array level is the array of fuel pins comprising an assembly. Therefore, an optimum pitch search would alter the spacing between the fuel pins within the assembly. The spacing can be expanded until the array intersects the first region external to it. The exterior size of the fuel pin array would grow or shrink within the confines of the exterior region (fuel assembly shroud). If the external regions are described using replicate regions, the array can grow or shrink within the confines of the maximum and minimum constraints.

If replicate regions are used outside an altered region or an array whose spacing units are altered, the dimensions of the replicate regions are recalculated (maintaining the thickness) at each search pass without having to enter search data for those regions. However, geometry regions specified by a geometry shape (sphere, cuboid, cylinder, etc.) that exist outside an altered region or an array whose spacing units are being altered will remain unchanged unless search data are provided for them. In other words, REPLICATE regions will grow and shrink in response to changes in the dimensions of the interior region, but other geometry shapes will not.

Some of the limitations applicable to a pitch or dimension search are:

1. A pitch search is performed only at the lowest array level unless search commands are entered to keep the lowest array level unit unchanged and other commands are entered to cause other units to be altered.

2. A pitch search alters the spacing in either the X dimension for a slab, the X and Y dimensions for an array of cylinders, or the X Y and Z dimensions for an array of spheres. Entering a search constant of zero for +X, X, +Y, Y, +Z, and/or Z will keep the corresponding dimension from being altered.

3. A pitch search alters only the outer region of the unit(s) used in the array at the lowest array level unless the search data specifying otherwise is input.

4. A search cannot alter a region whose boundaries are set by the code (i.e., an ARRAY, CORE BOUNDARY, or REPLICATE following an ARRAY). If the dimensions of a replicate region are to be altered, the dimensions of the region interior to it must be explicitly defined. For example, the interior region can be a standard geometry shape (sphere, cylinder, cuboid, etc.), but cannot be a replicate following an array or core boundary.

5. All searches allow auxiliary search data.

Concentration searches can also be performed using CSAS5S. A concentration search alters only those standard compositions specified in the search data. Care must be taken when searching on standard compositions beginning with SOLN, ATOM, WTPT, or ARBM (predecessor to ATOM and WTPT in earlier SCALE versions). One or more of their components can be altered but this will not directly affect the other components. For example, if the standard composition component name specified in the material information data is SOLN (SOLNUO2F2) and the concentration search data specifies SCNAME=UO2F2, the amount of uranyl fluoride salt, UO2F2, in the solution will be altered,

but the amount of water and hydrofluoric acid in the solution will remain unchanged. Therefore, the resultant mixture may no longer meet the criteria for a solution (SOLN) specification.

Physically, the concentration can vary from zero to some upper limit. The code will prevent the concentration from falling below zero, but the user is responsible for setting constraints that prevent the concentration from exceeding reasonable values. The theoretical density is a reasonable upper limit.

8.6 Optimum pitch search

An optimum pitch search searches for the pitch that yields the highest value of k_{eff} An optimum pitch search is activated by entering "OPTIMUM PITCH" in the search data. By default, the search is performed at the lowest array level and only the spacing in the X-direction for slabs, the X and Y-directions for cylindrical arrays, and the X, Y, and Z-directions for spherical arrays. The search constants are defaulted to 1.0 for the applicable +X, X, +Y, Y, +Z, and Z dimensions of the outermost region. The dimensions of other geometry regions will not be changed (their search constants are defaulted to 0.0) unless additional search data containing appropriate instructions are supplied.

The limits for an optimum pitch search can be set using either the MAXPITCH= and MINPITCH= options in the optional search parameters or the +CON= and CON= options in the search parameter constraints of the auxiliary search commands. MAXPITCH= and MINPITCH= are used to enter a value of the maximum allowed pitch and minimum allowed pitch respectively. +CON= and CON= are used to enter values for the parameter constraints (i.e., the maximum and minimum allowed value of the search parameter). Typically, it is easier to set the maximum allowed pitch and minimum allowed pitch using MAXPITCH= and MINPITCH= than it is to calculate the value of the parameter corresponding to those pitches. The default minimum constraint corresponds to MINPITCH, the pitch at which the largest interior region of a unit used in the array is in contact with the spacing cuboid of that unit. The maximum constraint is defaulted to 5 times the minimum constraint. In the first search pass, the code calculates k_{eff} for the initial problem geometry. The next two passes calculate the k_{eff} for the dimensions corresponding to the minimum constraint and maximum constraint. Subsequent passes fit the previous results to a cubic equation to select new dimensions.

Consider a $10 \times 10 \times 10$ array of uranium spheres surrounded by water having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the $10 \times 10 \times 10$ array is defined to be array 1. Search data and results for some optimum pitch searches using this example are given in inputs 1 through 6 below.

8.6.1 Default Search — Array of Centered Spheres

This problem contains search data for a default optimum pitch search. The problem consists of a $10 \times 10 \times 10$ array of uranium spheres surrounded by low density water. The spheres are 90% ^{235}U and 10% ^{238}U and have a radius of 2.0 cm. The spheres are originally centered on an 8.0 cm X, Y, and Z pitch with interstitial low density (0.01 gm/cc) water. The problem searches for the pitch that will produce the maximum k_{eff} for the system.

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
D
E
F
A
U
L
T
P
I
T
C
H
```

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```
V7
-238

R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
I
C
E
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```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

S
P
H
E
R
E  1 1 2
.0

C
U
B
O
I
D  2 1 6
P4
.0

E
N
D
G
E
O
M
E
T
R
Y
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```
R
E
A
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A
R
R
A
Y

A
R
A
=1
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X
=10
N
U
Y
=10
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U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A
```

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```
R
E
A
D
S
E
A
```

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```
E
N
D
```

This data will cause the code to alter the +X, X, +Y, Y, +Z, and Z dimensions of the outer region of unit 1 and search for the dimensions that give the maximum k_{eff}. Because the next to last outer dimension of the unit contained in the array are spheres, all six dimensions are altered. The original relationship between the dimensions is preserved (i.e., the original ratio of the X to Y to Z dimensions of the cuboid is preserved throughout the search). Because this is an optimum pitch search, the sphere dimensions will not be changed. For this particular example, results for six passes are given. A final search results for the problem follow:

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*
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*
*
s
e
a
r
c
h
p
a
s
s  1
k
e
f
f
=  5
.05769
E
-01
+
o
r
-  1
.10681
E
-03
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*
*
*
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*
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```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

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*
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*
*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
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t
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a
s
s  2
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f
f
=  1
.28382
E
+00
+
o
r
-  1
.70155
E
-03
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k
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=  2
.58700
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-01
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-  8
.16664
E
-04
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s  4
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.86712
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-  8
.92672
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a
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a
m
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w
a
s  1.25000E+00

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c
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a
s
s  5
k
e
f
f
=  2
.66952
E
-01
+
o
r
-  8
.42503
E
-04
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t
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v
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h
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*
s
e
a
r
c
h
p
a
s
s   6
k
e
f
f
=   2
.63611
E
-01
+
o
r
-   7
.74438
E
-04
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```
t
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p
a
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a
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e
t
e
r
w
a
s  2.16471E+00
1                                        10
x10
x10
a
r
r
a
y
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a
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r
c
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c
o
n
v
e
r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  2
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -5.00000E-0

t
h
e
e
q
u
a
t
i
o
n
u
s
e
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n
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```
k
-
e
f
f
=
+6
.69365
E
-01
-7
.39837
E
-01
*
p
+4
.33577
E
-01
*
p
*
*2
-8
.22064
E
-02
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  1
.28382
E
+00
+
o
r
-  1
.70155
E
-03
t
h
e
c
o
r
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m
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d
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a
b
i
a
s
g
e
o
m
e
t
r
y
d
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s
c
r
i
p
t
i
o
n
f
o
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s
e
u
n
i
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u
t
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l
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z
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r
e
g
i
o
n
n
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m
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-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
= 2
.0000
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
```

(continues on next page)

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```
 2
c
u
b
o
i
d   2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 2
.0000
-
y
=
-2
.0000
+
z
= 2
.0000
-
z
=
-2
.0000

*
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8.6.2 Default Search — Array of Off-Centered Spheres

This is the same problem as described above except the spheres are now off-centered in the X and Y dimensions. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
D
E
F
A
U
L
T
P
I
T
C
H
S
E
A
R
C
H
-
O
F
F
S
E
T

V7
-238

R
E
A
D
C
O
M
P

U
R
```

(continues on next page)

```
A
N
I
U
M 1 1
.0  300
.0 92235 90
```

(continued from previous page)

```
H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
P
H
S
Q
U
A
R
E
P
P
I
T
C
H
=8
.0 2
F
U
E
L
D
=4
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

S
P
H
E
R
E  1 1 2
.0

C
U
B
O
I
D  2 1 6
.0
-2
.0  3
.0
-5
.0  4
.0
-4
.0

E
N
D
G
E
O
M
E
T
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A

R
E
A
D
S
E
A
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N
D
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*
s
e
a
r
c
h
p
a
s
s  1
k
e
f
f
=  5
.06585
E
-01
+
o
r
-  1
.12636
E
-03
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t
h
e
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a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

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*m
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k
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v
d
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t
a
h
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b
e
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n
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s
s  2
k
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f
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=  1
.28382
E
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.70155
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a
s
s  3
k
e
f
f
=  2
.58916
E
-01
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o
r
-  8
.16022
E
-04
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v
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t
a
h
a
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p
a
s
s  4
k
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f
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=  2
.87506
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-01
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-  8
.38203
E
-04
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e
p
a
r
a
m
e
t
e
r
w
a
s  1.25000E+00

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b
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t 95
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s
e
a
r
c
h
p
a
s
s  5
k
e
f
f
=  2
.67987
E
-01
+
o
r
-  8
.48127
E
-04
*
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t
e
r
w
a
s  1.95962E+00

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e
d
k
e
n
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v
d
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a
h
a
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b
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n
r
e
w
r
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t
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t 95
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```

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*
*
s
e
a
r
c
h
p
a
s
s  6
k
e
f
f
=  2
.64640
E
-01
+
o
r
-  7
.99055
E
-04
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```

(continues on next page)

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  2.15903E+00
                                10
x10
x10
a
r
r
a
y
d
e
f
a
u
l
t
p
i
t
c
h
s
e
a
r
c
h
-
o
f
f
s
e
t

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*
```

(continues on next page)

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
c
o
n
v
e
r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  2
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -5.00000E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

(continued from previous page)

```
k
-
e
f
f
=
+6
.69265
E
-01
-7
.40343
E
-01
*
p
+4
.35409
E
-01
*
p
*
*2
-8
.28404
E
-02
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  1
.28382
E
+00
+
o
r
-  1
.70155
E
-03
t
h
e
c
o
r
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e  1  1
r
a
d
i
u
s
= 2
.0000
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
( 0
.0000
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d  2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 2
.0000
-
y
=
-2
.0000
+
z
= 2
.000
-
z
=
-2
.0000

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

8.6.3 Array of Centered Spheres — Constant Z Spacing

This is the same problem as the first problem described above except the array does not change in the Z dimensions. This is done by using MORE and specifying a KEEP command. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
D
E
F
A
U
L
T
P
I
T
C
H
S
E
A
R
C
H
-
C
H
A
N
G
E
I
N
X
&
Y
O
N
L
Y

V7
-238

R
E
A
D
C
O
M
P
```

(continues on next page)

(continued from previous page)

```
U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
P
H
S
Q
U
A
R
T
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

S
P
H
E
R
E  1 1 2
.0

C
U
B
O
I
D  2 1 6
P4
.0

E
N
D
G
E
O
M
E
T
R
Y
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A
```

(continues on next page)

```
R
E
A
D
S
E
A
```

(continued from previous page)

```
K
E
E
P
U
N
I
T
=1
R
E
G
=2
+
Z
=1
.0
-
Z
=1
.0

E
N
D
S
E
A
R
C
H

E
N
D
```

```
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```

(continues on next page)

```
s
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a
r
c
h
p
```

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

*
*
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*
*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t 95
*
*
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```

(continues on next page)

(continued from previous page)

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s
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p
a
s
s  2
k
e
f
f
=  9
.06304
E
-01
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o
r
-  1
.57239
E
-03
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t
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s
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a
s
s  3
k
e
f
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=  2
.82956
E
-01
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.20501
E
-04
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t
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e
t
e
r
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a
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t 95
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s
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a
r
c
h
p
a
s
s  4
k
e
f
f
=  3
.19086
E
-01
+
o
r
-  9
.27655
E
-04
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t
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v
d
a
t
a
h
a
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b
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n
r
e
w
r
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t 95
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```

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s
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a
r
c
h
p
a
s
s  5
k
e
f
f
=  2
.94889
E
-01
+
o
r
-  8
.49552
E
-04
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```

(continues on next page)

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  1.91631E+00
                        10
x10
x10
a
r
r
a
y
d
e
f
a
u
l
t
p
i
t
c
h
s
e
a
r
c
h
-
c
h
a
n
g
e
i
n
x
&
y
o
n
l
y
```

(continues on next page)

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
c
o
n
v
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c
e
w
a
s
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c
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d
o
n
p
a
s
s  2
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -5.00000E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

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```
k
-
e
f
f
=
+5
.70750
E
-01
-4
.42912
E
-01
*
p
+2
.39464
E
-01
*
p
*
*2
-4
.35513
E
-02
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  9
.06304
E
-01
+
o
r
-  1
.57239
E
-03
t
h
e
c
o
r
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e  1  1
r
a
d
i
u
s
= 2
.0000
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
( 0
.0000
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d  2  1
+
x
= 2
.0000
-
x
=
-2
.000
+
y
= 2
.0000
-
y
=
-2
.0000
+
z
= 4
.0000
-
z
=
-4
.0000

*
*
*
```

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```
*
*
*
```

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8.6.4 Default Search — Array of Centered Cylinders

This problem contains search data for a default optimum pitch search. The problem consists of a 10 × 10 × 10 array of uranium cylinders surrounded by low density water. The cylinders are 90% ^{235}U and 10% ^{238}U and have a radius of 2.0 cm and a length of 20 cm. The cylinders are originally centered on an 8.0 cm X and Y pitch and a 24 cm Z pitch with interstitial low density (0.01 gm/cc) water. The problem searches for the pitch that will produce the maximum k_{eff} for the system. Because this is an array of cylinders, by default only the X and Y dimensions are modified during the search. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
D
E
F
A
U
L
T
P
I
T
C
H
S
E
A
R
C
H
-
C
H
A
N
G
E
I
N
X
&
Y
O
N
L
Y

V7
-238
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

C
Y
L
I
N
D
E
R  1 1 2
.0  10
.0
-10
.0

C
U
B
O
I
D  2 1 4
p4
.0  2
p12
.0

E
N
D
G
E
O
M
E
T
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A
```

(continues on next page)

```
R
E
A
D
S
E
A
```

(continued from previous page)

```
E
N
D
S
E
A
R
C
H

E
N
D
```

```
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*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
s
e
a
r
c
h
p
a
s
s  1
k
e
f
f
=  1
.09882
E
+00
+
o
r
-  1
.75627
E
-03
*
*
*
*
```

(continues on next page)

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

*
*
*
*
*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t 95
*
*
*
```

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(continued from previous page)

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*
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*
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*
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*
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*
*
*
*
*
s
e
a
r
c
h
p
a
s
s  2
k
e
f
f
=  1
.66591
E
+00
+
o
r
-  1
.93770
E
-03
*
*
*
*
*
*
*
*
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*
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*
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*
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```

(continues on next page)

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s -5.00000E-01

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*
*
*
*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t 95
*
*
*
```

(continues on next page)

(continued from previous page)

```
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*
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*
*
*
*
*
*
*
*
*
*
*
s
e
a
r
c
h
p
a
s
s  3
k
e
f
f
=  5
.08235
E
-01
+
o
r
-  1
.28586
E
-03
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
```

(continues on next page)

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  2.50000E+00

*
*
*
*
*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t
*
*
*
```

(continues on next page)

(continued from previous page)

```
*
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*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
s
e
a
r
c
h
p
a
s
s  4
k
e
f
f
=  6
.33884
E
-01
+
o
r
-  1
.28582
E
-03
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
```

(continues on next page)

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  1.25000E+00
                        10
x10
x10
a
r
r
a
y
d
e
f
a
u
l
t
p
i
t
c
h
s
e
a
r
c
h
-
c
h
a
n
g
e
i
n
x
&
y
o
n
l
y
```

(continues on next page)

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
c
o
n
v
e
r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  2
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -5.00000E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

(continued from previous page)

```
k
-
e
f
f
=
+1
.09882
E
+00
-8
.48276
E
-01
*
p
+5
.17313
E
-01
*
p
*
*2
-1
.08998
E
-01
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  1
.66591
E
+00
+
o
r
-  1
.93770
E
-03
t
h
e
c
o
r
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t     1
-
-
-
-
-
 1
c
y
l
i
n
d
e
r  1  1
r
a
d
i
u
s
= 2
.0000
+
z
= 10
.000
-
z
=
-10
.000
c
e
n
t
e
r
l
i
n
e
i
s
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d    2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 2
.0000
-
y
=
-2
.0000
+
z
= 12
.000
-
z
=
-12
.000

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

8.6.5 Array of Centered Cylinders — Search Extended to Z Dimension

This is the same problem as given above except the search has been extended to include the Z dimension. The input data causes the code to alter the +X, X, +Y, Y, +Z, and Z dimensions of the outer region of unit 1 and search for the dimensions that give the maximum *keff*. The +Z and Z search constants were chosen to maintain the same spacing between cylinder surfaces in the X, Y and Z dimensions throughout the search. Because this is an optimum pitch search, the cylinder dimensions will not be changed. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
D
E
F
A
U
L
T
P
I
T
C
H
S
E
A
R
C
H
-
C
H
A
N
G
E
I
N
X
,
Y
,
Z

V7
-238
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

C
Y
L
I
N
D
E
R  1 1 2
.0  10
.0
-10
.0

C
U
B
O
I
D  2 1 4
p4
.0  2
p12
.0

E
N
D
G
E
O
M
E
T
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A
```

(continues on next page)

```
R
E
A
D
S
E
A
```

(continued from previous page)

```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=2
+
Z
=0
.33333
-
Z
=0
.33333

E
N
D
S
E
A
R
C
H

E
N
D
```

```
*
*
*
*
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*
*
*
*
```

(continues on next page)

```
*
s
e
a
r
c
h
```

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

*
*
*
*
*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t 95
*
*
*
```

(continues on next page)

(continued from previous page)

```
*
*
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*
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*
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*
*
*
*
*
*
*
*
*
*
*
s
e
a
r
c
h
p
a
s
s  2
k
e
f
f
=  1
.77881
E
+00
+
o
r
-  1
.79505
E
-03
*
*
*
*
*
*
*
*
*
*
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*
*
*
*
*
*
*
*
*
*
*
```

(continues on next page)

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s -5.00000E-01

*
*
*
*
*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t 95
*
*
*
```

(continues on next page)

(continued from previous page)

```
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*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
s
e
a
r
c
h
p
a
s
s  3
k
e
f
f
=  4
.54894
E
-01
+
o
r
-  1
.09005
E
-03
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
*
```

(continues on next page)

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  2.50000E+00

*
*
*
*
*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t
95
*
*
*
```

(continues on next page)

(continued from previous page)

```
*
*
*
*
*
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*
*
*
*
*
*
*
*
*
*
*
*
*
*
s
e
a
r
c
h
p
a
s
s  4
k
e
f
f
=  5
.70747
E
-01
+
o
r
-  1
.32088
E
-03
*
*
*
*
*
*
*
*
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*
*
*
*
*
*
*
*
*
*
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*
*
*
*
```

(continues on next page)

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  1.25000E+00
                          10
x10
x10
a
r
r
a
y
d
e
f
a
u
l
t
p
i
t
c
h
s
e
a
r
c
h
-
c
h
a
n
g
e
i
n
x
,
y
,
z
*
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*
*
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*
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*
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(continues on next page)

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```
*
*
*
```

(continued from previous page)

```
c
o
n
v
e
r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  2
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -5.00000E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

(continued from previous page)

```
k
-
e
f
f
=
+1
.09882
E
+00
-1
.00799
E
+00
*
p
+6
.36691
E
-01
*
p
*
*2
-1
.34609
E
-01
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  1
.77881
E
+00
+
o
r
-  1
.79505
E
-03
t
h
e
c
o
r
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
-
 1
c
y
l
i
n
d
e
r  1  1
r
a
d
i
u
s
= 2
.0000
+
z
= 10
.000
-
z
=
-10
.000
c
e
n
t
e
r
l
i
n
e
i
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d    2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 2
.0000
-
y
=
-2
.0000
+
z
= 10
.000
-
z
=
-10
.000

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

8.7 Minimum pitch search

A minimum pitch search searches for the pitch that yields the lowest value of *keff*. A minimum pitch search is activated by entering "MINIMUM PITCH" in the search data. By default, the search is performed at the lowest array level and only the spacing in the X-direction for slabs, the X and Y directions for cylindrical arrays, and the X, Y, and Z directions for spherical arrays. The search constants are defaulted to 1.0 for the applicable +X, X, +Y, Y, +Z, and Z dimensions of the outermost region. The dimensions of other geometry regions will not be changed (their search constants are defaulted to 0.0) unless additional search data containing appropriate instructions are supplied.

The limits for a minimum pitch search are the same as an optimum pitch search as described in the previous section.

8.7.1 Array of Centered Uranium Slabs

Consider a 10 × 1 × 1 array of uranium metal slabs. The uranium slabs are 2 cm in thick in the X dimension and 200 cm thick in the Y and Z dimensions. On each side of the uranium slab in the X dimension is 1 cm of H_2O, then 1 cm of Boral, then 1 cm of H_2O resulting in an initial center-to-center spacing is 8.0 cm. The slabs are 90% ^{235}U and 10% ^{238}U, the water is full density, and the Boral is 36.7% B_4C. The uranium slabs and their associated materials are defined to be unit 1, and the 10 × 1 × 1 array is defined to be array 1. A minimum pitch of 6.01 cm is specified, MINPITCH=6.01, and a maximum pitch of 14.0 cm is specified, MAXPITCH=14.0. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x1
x1
A
R
R
A
Y
D
E
F
A
U
L
T
P
I
T
C
H
S
E
A
R
C
H
-
S
L
A
B
```

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```
V7
-238

R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0   300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 1
.0   300
.0
E
N
D

B4
C     3 0
.367 300
.0
E
N
D

A
l      3 0
.633 300
.0
E
N
D

H2
O     4 1
.0   300
.0
E
N
D
```

(continues on next page)

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```
E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
Y
M
M
S
L
A
B
C
E
L
L
P
I
T
C
H
=8
.0 4
F
U
E
L
D
=2
.0 1
```

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```
C
L
A
D
D
=6
.01 3
G
A
P
D
=4
.0 2
E
N
D

E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

C
U
B
O
I
D  1 1 1
.0
-1
.0  4
P100
.0
```

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```
C
U
B
O
I
D  2 1 2
.0
-2
.0  4
P100
.0

C
U
B
O
I
D  3 1 3
.0
-3
.0  4
P100
.0

C
U
B
O
I
D  4 1 4
.0
-4
.0  4
P100
.0

E
N
D
G
E
O
M
E
T
R
Y

R
E
A
D
A
R
R
A
Y
```

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```
A
R
A
=1
N
U
X
=10
N
U
Y
=1
N
U
Z
=1
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A

R
E
A
D
S
E
A
R
C
H
M
I
N
I
M
U
M
```

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M
I
N
P
I
T
C
H
=6
.0
M
A
X
P
I
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=14
.0

E
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m
e
t
e
r
w
a
s  0.00000E+00

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s
s  2
k
e
f
f
=  1
.43116
E
+00
+
o
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-  1
.57018
E
-03
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t
e
r
w
a
s -2.50000E-01

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k
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v
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r
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c
h
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a
s
s  3
k
e
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=  8
.04815
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-01
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o
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-  1
.47600
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h
a
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r
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i
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*
s
e
a
r
c
h
p
a
s
s  4
k
e
f
f
=  9
.05346
E
-01
+
o
r
-  1
.47107
E
-03
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p
a
r
a
m
e
t
e
r
w
a
s  3.75000E-01
                                    10
x1
x1
a
r
r
a
y
d
e
f
a
u
l
t
p
i
t
c
h
s
e
a
r
c
h
-
s
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a
b

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c
o
n
v
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r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  3
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s   7.50000E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

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```
k
-
e
f
f
=
+1
.13755
E
+00
-9
.12964
E
-01
*
p
+9
.40907
E
-01
*
p
*
*2
-4
.20205
E
-01
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  8
.04815
E
-01
+
o
r
-  1
.47600
E
-03
t
h
e
c
o
r
```

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```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

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```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
-
 1
c
u
b
o
i
d    1  1
+
x
= 1
.0000
-
x
=
-1
.0000
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d    2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00
 3
c
u
b
o
i
d    3  1
+
x
= 3
.0000
-
x
=
-3
.0000
+
y
= 100
.00
-
y
=
```

(continues on next page)

```
-100
.00
+
z
= 100
.00
-
```

(continued from previous page)

```
 4
c
u
b
o
i
d    4  1
+
x
= 7
.0000
-
x
=
-7
.0000
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00

*
*
*
```

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```
*
*
*
```

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8.8 Critical pitch search

A critical pitch search alters the outer region of the unit or units at the lowest array level in search of a specified value of k_{eff}. A critical pitch search is activated by entering "CRITICAL PITCH" in the search data. By default, the search is performed at the lowest array level, and only the spacing in the X and Y directions (the X and Y dimensions of the outermost region of the unit(s) used in the array at the lowest array level) will be changed. The search constants are defaulted to 1.0 for the +X, X, +Y, and Y dimensions of the region. The dimensions of other geometry regions will not be changed (their search constants are defaulted to 0.0) unless additional search data containing appropriate instructions are supplied.

The limits for a critical pitch search can be set using either MAXPITCH= and MINPITCH= in the optional search parameters or +CON= and CON= in the search parameter constraints of the auxiliary search commands. MAXPITCH= and MINPITCH= are used to enter a value of the maximum allowed pitch and minimum allowed pitch respectively. Parameters +CON= and CON= are used to enter values for the parameter constraints (i.e., the maximum and minimum allowed value of the search parameter). Typically, it is easier to set the maximum allowed pitch and minimum allowed pitch using MAXPITCH= and MINPITCH= than it is to calculate the value of the parameter corresponding to those pitches. The default minimum constraint corresponds to MINPITCH, the pitch at which the largest interior region of a unit used in the array is in contact with the spacing cuboid of that unit. The maximum constraint is defaulted to 5 times the minimum constraint. The code calculates k_{eff} for the initial geometry first. Then the dimensions corresponding to the minimum constraint and maximum constraint are calculated.

8.8.1 Default Search — Array of Centered Spheres

This problem contains search data for a default critical pitch search with k_{eff} specified to be 0.95. The problem consists of a 10 × 10 × 10 array of uranium spheres surrounded by low density water. The spheres are 90% ^{235}U and 10% ^{238}U and have a radius of 2.0 cm. The spheres are originally centered on an 8.0 cm X, Y, and Z pitch with interstitial low density (0.01 gm/cc) water. The problem searches for the pitch that will produce a k_{eff} = 0.95 for the system.

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
D
E
F
A
U
L
T
P
I
T
C
H
S
E
A
R
C
H
```

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```
V7
-238

R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
I
C
E
```

(continues on next page)

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```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

S
P
H
E
R
E  1 1 2
.0

C
U
B
O
I
D  2 1 6
P4
.0

E
N
D
G
E
O
M
E
T
R
Y
```

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```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A

R
E
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E
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N
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r
c
h
p
a
s
s  1
k
e
f
f
=  5
.05769
E
-01
+
o
r
-  1
.10681
E
-03
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t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

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*m
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e
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k
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n
o
v
d
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t
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h
a
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=  2
.58700
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.16664
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a
s
s  3
k
e
f
f
=  1
.28382
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+00
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o
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-  1
.70155
E
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k
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f
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=  8
.08580
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-01
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-  1
.54692
E
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p
a
s
s  5
k
e
f
f
=  9
.37897
E
-01
+
o
r
-  1
.63624
E
-03
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k
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v
d
a
t
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h
a
s
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r
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w
r
i
t
t
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o
n
u
n
i
t 95
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```

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*
s
e
a
r
c
h
p
a
s
s  6
k
e
f
f
=  9
.49167
E
-01
+
o
r
-  1
.64684
E
-03
*
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```

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```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s -3.79251E-01
                                        10
x10
x10
a
r
r
a
y
d
e
f
a
u
l
t
p
i
t
c
h
s
e
a
r
c
h

*
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```

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```
*
*
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```

(continued from previous page)

```
c
o
n
v
e
r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  6
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -3.79251E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

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```
k
-
e
f
f
=
+5
.33889
E
-01
-9
.31824
E
-02
*
p
+2
.29294
E
+00
*
p
*
*2
-9
.20141
E
-01
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  9
.49167
E
-01
+
o
r
-  1
.64684
E
-03
t
h
e
c
o
r
```

(continues on next page)

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```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
= 2
.0000
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   2  1
+
x
=  2
.4830
-
x
=
-2
.4830
+
y
= 2
.4830
-
y
=
-2
.4830
+
z
= 2
.4830
-
z
=
-2
.4830

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
                                        10
x10
x10
a
r
r
a
y
d
e
f
a
u
l
t
p
i
t
c
h
s
e
a
r
c
h

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
b
a
s
e
d
o
n
t
h
e
p
r
e
c
e
d
i
n
g
d
a
t
a
,
t
h
e
b
e
s
t
e
s
t
i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s   -3.79602E-01
```

(continues on next page)

(continued from previous page)

```
t
h
e
g
e
o
m
e
t
r
y
c
o
r
r
e
s
p
o
n
d
i
n
g
t
o
t
h
i
s
p
a
r
a
m
e
t
e
r
f
o
l
l
o
w
s
:

m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e  1  1
r
a
d
i
u
s
= 2
.0000
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d  2  1
+
x
= 2
.4816
-
x
=
-2
.4816
+
y
= 2
.4816
-
y
=
-2
.4816
+
z
= 2
.4816
-
z
=
-2
.4816

*
*
*
```

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```
*
*
*
```

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8.8.2 Array of Centered Cylinders — Search Extended to Z Dimension

This problem contains search data for a default critical pitch search with k_{eff} specified to be 0.95. The problem consists of a 10 × 10 × 10 array of uranium cylinders surrounded by low density water. The cylinders are 90% ^{235}U and 10% ^{238}U and have a radius of 2.0 cm and a length of 20 cm. The cylinders are originally centered on an 8.0 cm X and Y pitch and a 24 cm Z pitch with interstitial low density (0.01 gm/cc) water. The problem searches for the pitch that will produce a k_{eff} = 0.95 for the system. Because this is an array of cylinders, by default only the X and Y dimensions are modified during the search. The +Z and Z search constants were included and chosen such that the same spacing is maintained between cylinder surfaces in the X, Y and Z dimensions throughout the search. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
D
E
F
A
U
L
T
P
I
T
C
H
S
E
A
R
C
H
-
C
H
A
N
G
E
I
N
X
,
Y
,
Z

V7
-238
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

C
Y
L
I
N
D
E
R  1 1 2
.0  10
.0
-10
.0

C
U
B
O
I
D  2 1 4
p4
.0  2
p12
.0

E
N
D
G
E
O
M
E
T
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A

R
E
A
D
S
E
A
```

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```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=2
+
Z
=0
.33333
-
Z
=0
.33333

E
N
D
S
E
A
R
C
H

E
N
D
```

```
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```
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s
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a
r
c
h
```

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t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

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*
*m
o
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i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t 95
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s
e
a
r
c
h
p
a
s
s  2
k
e
f
f
=  1
.77881
E
+00
+
o
r
-  1
.79505
E
-03
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a
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e
t
e
r
w
a
s -5.00000E-01

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*m
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i
f
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e
d
k
e
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v
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a
h
a
s
b
e
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n
r
e
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r
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t 95
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*
s
e
a
r
c
h
p
a
s
s  3
k
e
f
f
=  1
.00616
E
+00
+
o
r
-  1
.61956
E
-03
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t
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p
a
r
a
m
e
t
e
r
w
a
s  1.09424E-01

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*m
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e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t 95
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```

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*
*
*
s
e
a
r
c
h
p
a
s
s  4
k
e
f
f
=  9
.48455
E
-01
+
o
r
-  1
.66901
E
-03
*
*
*
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*
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*
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```

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(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  1.91336E-01
                          10
x10
x10
a
r
r
a
y
d
e
f
a
u
l
t
p
i
t
c
h
s
e
a
r
c
h
-
c
h
a
n
g
e
i
n
x
,
y
,
z
```

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```
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```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
c
o
n
v
e
r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  4
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s   1.91336E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

(continued from previous page)

```
k
-
e
f
f
=
+1
.09882
E
+00
-9
.31106
E
-01
*
p
+7
.86483
E
-01
*
p
*
*2
-1
.42575
E
-01
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  9
.48455
E
-01
+
o
r
-  1
.66901
E
-03
t
h
e
c
o
r
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t     1
-
-
-
-
-
 1
c
y
l
i
n
d
e
r  1  1
r
a
d
i
u
s
= 2
.0000
+
z
= 10
.000
-
z
=
-10
.000
c
e
n
t
e
r
l
i
n
e
i
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d    2  1
+
x
= 4
.7653
-
x
=
-4
.7653
+
y
= 4
.7653
-
y
=
-4
.7653
+
z
= 12
.765
-
z
=
-12
.765

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
                                10
x10
x10
a
r
r
a
y
d
e
f
a
u
l
t
p
i
t
c
h
s
e
a
r
c
h
-
c
h
a
n
g
e
i
n
x
,
y
,
z

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
b
a
s
e
d
o
n
t
h
e
p
r
e
c
e
d
i
n
g
d
a
t
a
,
t
h
e
b
e
s
t
e
s
t
i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s    1.88950E-01
```

(continues on next page)

(continued from previous page)

```
t
h
e
g
e
o
m
e
t
r
y
c
o
r
r
e
s
p
o
n
d
i
n
g
t
o
t
h
i
s
p
a
r
a
m
e
t
e
r
f
o
l
l
o
w
s
:

m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t     1
-
-
-
-
-
-
 1
c
y
l
i
n
d
e
r  1  1
r
a
d
i
u
s
= 2
.0000
+
z
= 10
.000
-
z
=
-10
.000
c
e
n
t
e
r
1
1
n
e
i
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d    2  1
+
x
=  4
.7558
-
x
=
-4
.7558
+
y
=  4
.7558
-
y
=
-4
.7558
+
z
=  12
.756
-
z
=
-12
.756

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

8.8.3 Array of Centered Uranium Slabs

Consider a 10 × 1 × 1 array of uranium metal slabs. The uranium slabs are 2 cm thick in the X dimension and 200 cm thick in the Y and Z dimensions. On each side of the uranium slab in the X dimension is 1 cm of H_2O, then 1 cm of Boral, then 1 cm of H_2O resulting in an initial center-to-center spacing of 8.0 cm. The slabs are 90% ^{235}U and 10% ^{238}U, the water is full density, and the Boral is 36.7% B_4C. The uranium slabs and their associated materials are defined to be unit 1, and the 10 × 1 × 1 array is defined to be array 1. A minimum pitch of 6.0 cm is specified, MINPITCH=6.0, and a maximum pitch of 14.0 cm is specified, MAXPITCH=14.0. The code searches for the default value of k_{eff}. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x1
x1
A
R
R
A
Y
D
E
F
A
U
L
T
P
I
T
C
H
S
E
A
R
C
H
-
S
L
A
B

V7
-238

R
E
A
D
C
O
M
P
```

(continues on next page)

(continued from previous page)

```
U
R
A
N
I
U
M 1 1
.0   300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 1
.0   300
.0
E
N
D

B4
C     3 0
.367 300
.0
E
N
D

A
l      3 0
.633 300
.0
E
N
D

H2
O     4 1
.0   300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
```

(continues on next page)

(continued from previous page)

```
L
A
T
T
I
C
E
C
E
L
L
S
Y
M
M
S
L
A
B
C
E
L
L
P
I
T
C
H
=8
.0 4
F
U
E
L
D
=2
.0 1

C
L
A
D
D
=6
.0 3
G
A
P
D
=4
.0 2
E
N
D

E
N
D
C
E
L
L
D
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
G
E
O
M
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.13755
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.08380
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.68867
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-01
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.81717
E
-01
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.97707
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b
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i
d   1  1
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= 1
.0000
-
x
=
-1
.0000
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y
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.00
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=
-100
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z
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z
=
-100
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x
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-
x
=
-2
.0000
+
y
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.00
-
y
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-100
.00
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z
= 100
.00
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z
=
-100
.00
 3
c
u
b
o
i
d   3  1
+
x
= 3
.0000
-
x
=
-3
.0000
+
y
= 100
.00
-
y
=
```

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```
-100
.00
+
z
= 100
.00
-
```

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```
 4
c
u
b
o
i
d   4  1
+
x
= 4
.7573
-
x
=
-4
.7573
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
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                                    10
x1
x1
a
r
r
a
y
d
e
f
a
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t
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t
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m
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a
m
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t
e
r
i
s     1.85414E-01
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t
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r
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u
n
i
t     1
-
-
-
-
-
-
 1
c
u
b
o
i
d   1  1
+
x
= 1
.0000
-
x
=
-1
.0000
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00
```

(continues on next page)

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```
 2
c
u
b
o
i
d   2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00
 3
c
u
b
o
i
d   3  1
+
x
= 3
.0000
-
x
=
-3
.0000
+
y
= 100
.00
-
y
=
```

(continues on next page)

```
-100
.00
+
z
= 100
.00
-
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```
 4
c
u
b
o
i
d   4  1
+
x
= 4
.7417
-
x
=
-4
.7417
+
y
= 100
.00
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y
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8.9 Optimum dimension search

An optimum dimension search searches for the geometry dimensions that yield the highest value of *keff*. An optimum dimension search is activated by entering "OPTIMUM DIMENSION" in the search data. There are no defaulted search data in a dimension search. The user must specify the dimensions to be changed and the manner in which they will be changed as described in the auxiliary search commands.

A dimension search is performed by altering the regions having nonzero search constants specified in the auxiliary search commands portion of the search data. By default, the search constants for every dimension in the problem are zero. Only those dimensions having a nonzero search constant are altered by the code.

By default, a dimension search sets the minimum constraint to 10E10 and the maximum constraint to +10E10. The relationship between the constraints and the search constants are given in (8.1) and (8.2). If the default values of the constraints are used, appropriate search constants must be calculated using these equations. It may be simpler to set the search constants to 1.0 and calculate the corresponding maximum and minimum constraints. Several dimension search examples are shown below.

8.9.1 Array of Centered Spheres — Search in X, Y, and Z Dimensions

Consider a 10 × 10 × 10 array of uranium spheres arranged in an array having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the 10 × 10 × 10 array is defined to be array 1. The constraints are set to be consistent with those of this optimum pitch search case. The search data and results for an optimum dimension search that alters the X, Y, and Z dimensions of region 2 of unit 1 are given as follows.

```
=CSAS5S
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x10
x10
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R
A
Y
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D
I
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O
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C
H

V7
-238
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```
R
E
A
D
C
O
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U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
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R
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P
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E  1 1 2
.0

C
U
B
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D  2 1 6
P4
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F
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F1
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.65737
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.89427
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i
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i
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k
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v
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a
h
a
s
b
e
e
n
r
e
w
r
i
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n
i
t 95
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```

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s
e
a
r
c
h
p
a
s
s   6
k
e
f
f
=   2
.63297
E
-01
+
o
r
-   8
.48658
E
-04
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```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  2.17436E+00
                                    10
x10
x10
a
r
r
a
y
-
d
i
m
e
n
s
i
o
n
s
e
a
r
c
h

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c
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w
a
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o
n
p
a
s
s  2
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -5.00000E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

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```
k
-
e
f
f
=
+6
.70283
E
-01
-7
.35957
E
-01
*
p
+4
.26318
E
-01
*
p
*
*2
-7
.98562
E
-02
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  1
.28075
E
+00
+
o
r
-  1
.89662
E
-03
t
h
e
c
o
r
```

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```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
= 2
.0000
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 2
.0000
-
y
=
-2
.0000
+
z
= 2
.0000
-
z
=
-2
.0000

*
*
*
```

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```
*
*
*
```

(continued from previous page)

These MORE search data will cause the code to alter the +X, X, +Y, Y, Z, and +Z dimensions of the outer region (region 2) of unit 1 and search for the dimensions that give the maximum k_{eff}. Since all the UNIT 1 outer dimensions are the same (4 or 4) and all the search constants are the same (ALL=1.0) the code will alter each dimension the same amount for a search pass thus preserving the original relationship between dimensions. Because this is an optimum pitch search, the sphere dimensions will not be changed. The optimum dimension for this problem is when the spheres touch as shown in the output data above.

8.9.2 Array of Centered Spheres — Search in X and Y Dimensions

This is the same problem as described above except the spacing is only varied in the X and Y dimensions. Since only changes in the X and Y dimensions of the outer region are desired, the +X, X, +Y, and Y search constants must be set. Since all dimensions are to change at the same rate and have the same initial value, the search constants for the changing surfaces must be the same. The +Z and Z search constants by default are zero so these dimensions will not change. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
-
X
&
Y
D
I
M
E
N
S
I
O
N
O
P
T
I
M
U
M
S
E
A
R
C
H

V7
-238
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
```

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```
E
N
D
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E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

S
P
H
E
R
E  1 1 2
.0

C
U
B
O
I
D  2 1 6
P4
.0

E
N
D
G
E
O
M
E
T
R
Y
```

(continues on next page)

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```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
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D
A
T
A
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```
R
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S
E
A
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A
L
T
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N
I
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=1
R
E
G
=2
+
X
=1
.0
-
X
=1
.0
+
Y
=1
.0
-
Y
=1
.0

-
C
O
N
=
-0
.5
+
C
O
N
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E
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a
s
s  3
k
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.82956
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-  8
.20501
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s
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r
c
h
p
a
s
s  4
k
e
f
f
=  3
.19086
E
-01
+
o
r
-  9
.27655
E
-04
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a
s  1.25000E+00

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a
h
a
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b
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t 95
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*
*
s
e
a
r
c
h
p
a
s
s  5
k
e
f
f
=  2
.94889
E
-01
+
o
r
-  8
.49552
E
-04
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```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  1.91631E+00
                                10
x10
x10
a
r
r
a
y
-
x
&
y
d
i
m
e
n
s
i
o
n
o
p
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i
m
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m
s
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```
c
o
n
v
e
r
g
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n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  2
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -5.00000E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

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```
k
-
e
f
f
=
+5
.70750
E
-01
-4
.42912
E
-01
*
p
+2
.39464
E
-01
*
p
*
*2
-4
.35513
E
-02
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  9
.06304
E
-01
+
o
r
-  1
.57239
E
-03
t
h
e
c
o
r
```

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```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

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(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
= 2
.0000
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
```

(continues on next page)

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 2
c
u
b
o
i
d   2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 2
.0000
-
y
=
-2
.0000
+
z
= 4
.0000
-
z
=
-4
.0000

*
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*
```

(continued from previous page)

```
*
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*
```

(continued from previous page)

8.9.3 Array of Offset Spheres — Search in X and Y Dimensions

This is the same problem as described above except the spheres are now off-centered in the X and Y dimensions. Since only changes in the X and Y dimensions of the outer region are desired, the +X, X, +Y, and Y search constants must be set. All dimensions are to change at the same rate but they have different initial values. The search constants specify how surfaces change relative to each other. For this case the search constants were chosen so that the moderator spacing for the X and Y dimensions will change at the same rate. The +Z and Z search constants by default are zero so these dimensions will not change.

The input data and the final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
-
X
&
Y
D
I
M
E
N
S
I
O
N
O
P
T
I
M
U
M
S
E
A
R
C
H
-
O
F
F
S
E
T
```

(continues on next page)

(continued from previous page)

```
V7
-238

R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
I
I
C
E
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

S
P
H
E
R
E  1 1 2
.0
O
R
I
G
I
N  2
.0  1
.0  0
.0

C
U
B
O
I
D  2 1 6
.0
-2
.0 5
.0
-3
.0 2
P 4
.0
```

(continues on next page)

(continued from previous page)

```
E
N
D
G
E
O
M
E
T
R
Y

R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y
```

(continues on next page)

(continued from previous page)

```
E
N
D
D
A
T
A

R
E
A
D
S
E
A
R
C
H
O
P
T
I
M
U
M
D
I
M
E
N
S
I
O
N
M
O
R
E

A
L
T
E
R
U
N
I
T
=1
R
E
G
=2
+
X
=0
.3333333
-
X
=1
.0
+
Y
```

(continues on next page)

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```
-
C
O
N
=
-1
.0
+
C
O
N
=5
.0

E
N
D
S
E
A
R
C
H

E
N
D
```

```
*
*
*
```

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

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*
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*m
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e
d
k
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v
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s
e
a
r
c
h
p
a
s
s  2
k
e
f
f
=  9
.05152
E
-01
+
o
r
-  1
.53983
E
-03
*
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t 95
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```

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-  8
.07313
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.39609
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```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  3.82730E+00
                                10
x10
x10
a
r
r
a
y
-
x
&
y
d
i
m
e
n
s
i
o
n
o
p
t
i
m
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a
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c
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w
a
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a
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e
v
e
d
o
n
p
a
s
s  2
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -1.00000E+00

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

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```
k
-
e
f
f
=
+5
.73236
E
-01
-2
.19195
E
-01
*
p
+5
.80895
E
-02
*
p
*
*2
-5
.19734
E
-03
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  9
.05152
E
-01
+
o
r
-  1
.53983
E
-03
t
h
e
c
o
r
```

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```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
= 2
.0000
t
h
e
c
e
n
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i
s
l
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c
a
t
e
d
a
t
(  2
.0000
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   2  1
+
x
= 4
.0000
-
x
=  0
.0000
+
y
= 3
.0000
-
y
=
-1
.0000
+
z
= 4
.0000
-
z
=
-4
.0000

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8.9.4 Array of Cylinders — Search in X, Y, and Z Dimensions

This is the same array of cylinder problem as described in the previous section, except the search is an optimum dimension search. Since changes in the X, Y, and Z dimensions of the outer region are desired, the +X, X, +Y, Y, +Z, and Z search constants must be set. The search data ALL=1.0 sets all the outer region search constants to 1.0. However, a constant ratio for the center-to-center spacing of the units in desired so the Z dimensions will need to be reset to a lower value of 0.333333. This will ensure that the Z dimensions change at 1/3 the rate of the X and Y dimensions relative to their initial values. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
,
O
P
T
I
M
U
M
D
I
M
E
N
S
I
O
N
S
E
A
R
C
H
-
M
A
I
N
T
A
I
N
C
-
T
O
-
C
P
A
C
I
```

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```
V7
-238

R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
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I
C
E
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```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

C
Y
L
I
N
D
E
R  1 1 2
.0  10
.0
-10
.0

C
U
B
O
I
D  2 1 4
p4
.0  2
p12
.0

E
N
D
G
E
O
M
E
T
```

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```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
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X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
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R
R
A
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E
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T
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R
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S
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A
```

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T
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R
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G
=2
A
L
L
=1
.0
+
Z
=0
.3333333
-
Z
=0
.3333333

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C
O
N
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-0
.5
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k
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a
s
s  3
k
e
f
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=  4
.54369
E
-01
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.10229
E
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a
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c
h
p
a
s
s  4
k
e
f
f
=  5
.67573
E
-01
+
o
r
-  1
.26038
E
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r
w
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                10
x10
x10
a
r
r
a
y
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o
p
t
i
m
u
m
d
i
m
e
n
s
i
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s
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c
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m
a
i
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a
i
n
c
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n
p
a
s
s  2
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -5.00000E-01

t
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s
e
d
i
n
t
h
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```
k
-
e
f
f
=
+1
.09882
E
+00
-1
.01312
E
+00
*
p
+6
.38864
E
-01
*
p
*
*2
-1
.34691
E
-01
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  1
.78193
E
+00
+
o
r
-  2
.12022
E
-03
t
h
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c
o
r
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m
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i
a
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g
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o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
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d
i
n
t
h
i
s
p
r
o
b
l
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```
r
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g
i
o
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n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
c
y
l
i
n
d
e
r    1   1
r
a
d
i
u
s
= 2
.0000
+
z
=   10
.000
-
z
=
-10
.000
c
e
n
t
e
r
l
i
n
e
i
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d     2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 2
.0000
-
y
=
-2
.0000
+
z
= 10
.000
-
z
=
-10
.000

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*
```

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```
*
*
*
```

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8.10 Minimum dimension search

A minimum dimension search searches for the geometry dimensions that yield the lowest value of k_{eff}. A minimum dimension search is activated by entering "MINIMUM DIMENSION" in the search data. There are no defaulted search data in a dimension search. The user must specify the dimensions to be changed and the manner in which they will be changed as described in the auxiliary search commands.

A dimension search is performed by altering the regions having nonzero search constants specified in the auxiliary search commands portion of the search data. By default, the search constants for every dimension in the problem are zero. Only those dimensions having a nonzero search constant are altered by the code.

By default, a dimension search sets the minimum constraint to 10E10 and the maximum constraint to +10E10. The relationship between the constraints and the search constants are given in (8.1). and (8.2). If the default values of the constraints are used, appropriate search constants must be calculated using these equations. In some cases it may be simpler to set the search constants to 1.0 and calculate the corresponding maximum and minimum constraints. Several dimension search examples are shown below.

8.10.1 Infinite Array of Fuel Bundles Separated by Flux Traps — Search in X and Y-Dimensions

The fuel bundles in this problem represent 17 × 17 PWR fuel assemblies. The fuel pins are smeared together, making a mixture 100. The fuel pins consist of 2.35 wt % ^{235}U having a diameter of 0.823 cm, zirconium cladding having an outer diameter of 0.9627 cm, and a pitch of 1.275 cm. The fuel bundle is represented as a 10.8375 cm × 10.8375 cm × 366 cm cuboid of mixture 100 surrounded by Boral and then water. The Boral has a density of 2.65 g/cm^3 and is composed of 35.17 wt % B_4C and 64.83 wt % Al. The fuel bundles are at a fixed pitch of 13.0 cm. The problem searches for the thickness of Boral that will produce the lowest system k_{eff}. The input data and the final search results for this problem follow:

```
=csas5s

a
r
r
a
y
o
f
f
u
e
l
b
u
n
d
l
e
s
w
i
t
```

(continues on next page)

```
h
f
l
u
x
t
r
```

(continued from previous page)

```
v7
-238
read
 comp

u
o2    1
.84 300
.  92235 2
.35 92238 97
.65 end

z
r     2 1 end

h2
o    3 1 end

b4
c    4
d
e
n
=2
.65 0
.3517 end

a
l     4
d
e
n
=2
.65 0
.6483 end

h2
o    5 1 end
end
 comp
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
q
u
a
r
e
p
i
t
```

(continues on next page)

(continued from previous page)

```
end
 celldata
read
 param
 far
=yes
 gen
=
2
0
3
 npg
=
1
0
0
0
 end
 param
read
 geom

g
l
o
b
a
l
u
n
i
t 1

c
u
b
o
i
d 100 1 4
p10
.8375 2
p183
.0

c
u
b
o
i
d   4 1 4
p11
.0    2
p183
.0

c
u
b
o
i
d   5 1 4
p13
.0    2
p183
```

(continues on next page)

(continued from previous page)

```
end
 geom
read
 bounds
 xfc
=mirror
 yfc
=mirror
 end
 bounds
end
 data
read
 search

 minimum
 dimension

 more

a
l
t
e
r
u
n
i
t
=1
r
e
g
=2
+
x
=1
.0
-
x
=1
.0
+
y
=1
.0
-
y
=1
.0

-
c
o
n
=
-0
.009
+
c
o
n
=0
.181818
```

(continues on next page)

(continued from previous page)

```
end
 search
end
```

```
*
*
*
*
*
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*
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*
*
*
*
*
*
s
e
a
r
c
h
p
a
s
s  1
k
e
f
f
=  7
.18665
E
-01
+
o
r
-  1
.69354
E
-03
*
*
*
*
*
*
*
*
```

(continues on next page)

```
*
*
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*
*
*
*
*
```

(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

*
*
*
*
x
s
d
r
n
p
m
m
e
s
h
i
n
t
e
r
v
a
l
s
*
*
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*
*
        4
m
e
s
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8.10.2 Two Uranium Slabs Separated by a Flux Trap — Search in +X Dimensions

This problem consists of two 90 wt % enriched uranium metal slabs separated by a flux trap. Each uranium slab is 3.0 cm thick. The spacing between the slabs is 4 cm. Between the slabs is a Boral plate at each slab surface and water in between the two Boral plates. This problem searches for the thickness of the Boral plates and separating water that produces the lowest system k_{eff}. The input data and the final search results for this problem follow:

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V7
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U
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.0 92235 90
.0 92238 10
.0
E
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C 2 0
.367 300
.0
E
N
D

A
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.633 300
.0
E
N
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H2
O 3 1
.0 300
.0
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T 1

C
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D 3 1 1
.0 0
.0 4
P100
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C
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x
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y
= 100
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-
y
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8.11 Critical dimension search

A critical dimension search searches for the geometry dimensions that yield a specified value of k_{eff}. A critical dimension search is activated by entering "CRITICAL DIMENSION" in the search data. No defaulted search data are in a dimension search. The user must specify the dimensions to be changed and the manner in which they will be changed.

A dimension search is performed by altering the regions having nonzero search constants specified in the individual search commands portion of the search data. By default, the search constants for every dimension in the problem are zero. Only those dimensions having a nonzero search constant are altered by the code.

By default, a dimension search sets the minimum constraint to 10E10 and the maximum constraint to +10E10. The relationship between the constraints and the search constants is given in (8.1) and (8.2). If the default values of the constraints are used, appropriate search constants must be calculated using these equations. It may be simpler to set the search constants to 1.0 and calculate the corresponding maximum and minimum constraints. Several critical dimension search examples are shown below.

8.11.1 Array of Centered Spheres — Search in X, Y, and Z Dimensions

Consider a 10 × 10 × 10 array of uranium spheres arranged in an array having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the 10 × 10 × 10 array is defined to be array 1. A critical dimension search is performed on the outer dimension of the cuboid that will produce a system k_{eff} of 1.0. In the MORE search data, All=1.0 on region 2 of unit 1 specifies all six surfaces of the cuboid change identically. The search constraints are set to search from a sphere center-to-center spacing of 4 cm to 20 cm. The search data and results are given below.

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.0 92235 90
.0 92238 10
.0
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H2
O     2 0
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x
=
-2
.3965
+
y
= 2
.3965
-
y
=
-2
.3965
+
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.3965
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z
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-2
.3965

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x10
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```
b
a
s
e
d
o
n
t
h
e
p
r
e
c
e
d
i
n
g
d
a
t
a
,
t
h
e
b
e
s
t
e
s
t
i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s   -4.00545E-01
```

(continues on next page)

(continued from previous page)

```
t
h
e
g
e
o
m
e
t
r
y
c
o
r
r
e
s
p
o
n
d
i
n
g
t
o
t
h
i
s
p
a
r
a
m
e
t
e
r
f
o
l
l
o
w
s
:

m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
=  2
.0000
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   2  1
+
x
= 2
.3978
-
x
=
-2
.3978
+
y
= 2
.3978
-
y
=
-2
.3978
+
z
= 2
.3978
-
z
=
-2
.3978

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

8.11.2 Array of Centered Spheres — Search in X, Y, and Z Dimensions

Consider a 10 × 10 × 10 array of uranium spheres arranged in an array having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the 10 × 10 × 10 array is defined to be array 1. A critical dimension search is performed on the radius of the uranium sphere that will produce a system k_{eff} of 1.0. In the MORE search data, RADIUS=1.0 on region 1 of unit 1 specifies the sphere's radius is to be altered. The search constraints are set to search from a radius of 0.5 cm to 4.0 cm. The search data and results are given below.

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
-
D
I
M
E
N
S
I
O
N
S
E
A
R
C
H

V7
-238

R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D
```

(continues on next page)

(continued from previous page)

```
H2
O      2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
P
H
S
Q
U
A
R
E
P
P
I
T
C
H
=8
.0 2
F
U
E
L
D
=4
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

S
P
H
E
R
E  1 1 2
.0

C
U
B
O
I
D  2 1 6
P4
.0

E
N
D
G
E
O
M
E
T
R
Y
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A

R
E
A
D
S
E
A
```

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```
A
L
T
E
R
U
N
I
T
=1
C
E
L
L
=1
R
E
G
=1
R
A
D
I
U
S
=1
.0

-
C
O
N
=
-0
.75
+
C
O
N
=1
.0

E
N
D
S
E
A
R
C
H

E
N
D
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*
*
s
e
a
r
c
h
p
a
s
s  1
k
e
f
f
=  5
.05364
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-01
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o
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-  1
.20323
E
-03
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t
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a
r
a
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e
t
e
r
w
a
s  0.00000E+00

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a
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e
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e
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r
i
t
t
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n
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a
s
s  2
k
e
f
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=  1
.79497
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+
o
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-  1
.93055
E
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d
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d
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h
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s
e
a
r
c
h
p
a
s
s  3
k
e
f
f
=  9
.91353
E
-01
+
o
r
-  1
.56062
E
-03
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a
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a
m
e
t
e
r
w
a
s  3.83555E-01

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c
h
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a
s
s  4
k
e
f
f
=  9
.97513
E
-01
+
o
r
-  1
.61171
E
-03
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t
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r
a
m
e
t
e
r
w
a
s  3.90304E-01
                                        10
x10
x10
a
r
r
a
y
-
d
i
m
e
n
s
i
o
n
s
e
a
r
c
h

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```

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c
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n
v
e
r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  4
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s   3.90304E-01

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

(continued from previous page)

```
k
-
e
f
f
=
+5
.05364
E
-01
+1
.84705
E
+00
*
p
-2
.10615
E
+00
*
p
*
*2
+1
.54871
E
+00
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  9
.97513
E
-01
+
o
r
-  1
.61171
E
-03
t
h
e
c
o
r
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
= 2
.7806
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   2  1
+
x
= 4
.0000
-
x
=
-4
.0000
+
y
= 4
.0000
-
y
=
-4
.0000
+
z
= 4
.0000
-
z
=
-4
.0000

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
                                        10
x10
x10
a
r
r
a
y
-
d
i
m
e
n
s
i
o
n
s
e
a
r
c
h

*
*
*
```

(continued from previous page)

```
b
a
s
e
d
o
n
t
h
e
p
r
e
c
e
d
i
n
g
d
a
t
a
,
t
h
e
b
e
s
t
e
s
t
i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s    3.93037E-01
```

(continues on next page)

(continued from previous page)

```
t
h
e
g
e
o
m
e
t
r
y
c
o
r
r
e
s
p
o
n
d
i
n
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t
o
t
h
i
s
p
a
r
a
m
e
t
e
r
f
o
l
l
o
w
s
:

m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
=  2
.7861
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   2  1
+
x
= 4
.0000
-
x
=
-4
.0000
+
y
= 4
.0000
-
y
=
-4
.0000
+
z
= 4
.0000
-
z
=
-4
.0000

*
*
*
```

(continued from previous page)

8.11.3 Array of Centered Cylinders — Search in X and Y Dimensions

This problem contains search data for a critical dimension search with k_{eff} specified to be 0.95. The problem consists of a 10 × 10 × 2 array of uranium cylinders surrounded by low density water. The cylinders are 90% ^{235}U and 10% ^{238}U and have a radius of 2.0 cm and a length of 20 cm. The cylinders are originally centered on an 8.0 cm X and Y pitch and a 24 cm Z pitch with interstitial low density (0.01 gm/cc) water. The problem searches for the cylinder center-to-center spacing that will produce a k_{eff} = 0.95 for the system. Because this is a dimension search, all search data must be specified. The +X, X, +Y, and Y search constants are specified as well as the CON and +CON search constraints. The search data is set up to alter the cylinder center-to-center spacing from 4.0 cm to 16.0 cm during the search. The MORE search data CELL=1 ties the search data to the first unit cell thus ensuring they change in unison properly modifying the cross-section processing. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x10
x2
A
R
R
A
Y
D
I
M
E
N
S
I
O
N
S
E
A
R
C
H
-
C
H
A
N
G
E
I
N
X
,
Y

V7
-238

R
E
A
D
C
O
M
P
```

(continues on next page)

(continued from previous page)

```
U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.01 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
Q
U
A
R
E
P
I
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

C
Y
L
I
N
D
E
R  1 1 2
.0  10
.0
-10
.0

C
U
B
O
I
D  2 1 4
p4
.0  2
p12
.0

E
N
D
G
E
O
M
E
T
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=2
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A
```

(continues on next page)

```
R
E
A
D
S
E
A
```

(continued from previous page)

```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=2
+
X
=1
.0
-
X
=1
.0
+
Y
=1
.0
-
Y
=1
.0
C
E
L
L
=1

-
C
O
N
=
-0
.5
+
C
O
N
=2
.0

E
N
D
S
E
A
R
C
H
```

(continues on next page)

(continued from previous page)

```
E
N
D
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s
e
a
r
c
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p
a
s
s  1
k
e
f
f
=  8
.48434
E
-01
+
o
r
-  1
.50137
E
-03
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```
t
h
e
p
a
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m
e
t
e
r
w
a
s  0.00000E+00

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*m
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d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
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b
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e
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r
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w
r
i
t
t
e
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o
n
u
n
i
t 99
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s  2
k
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f
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=  4
.22734
E
-01
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-  9
.98609
E
-04
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e
r
w
a
s  2.00000E+00

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t 99
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s
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a
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c
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a
s
s  3
k
e
f
f
=  1
.49380
E
+00
+
o
r
-  1
.81532
E
-03
*
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t
h
e
p
a
r
a
m
e
t
e
r
w
a
s -4.77172E-01

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*m
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x2
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a
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r
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s  -1.13412E-01

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k
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e
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f
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+8
.52892
E
-01
-6
.96099
E
-01
*
p
+1
.13262
E
+00
*
p
*
*2
-4
.46134
E
-01
*
p
*
*3


k
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f
f
e
c
t
i
v
e
=  9
.47041
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-01
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o
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-  1
.57053
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t      1
-
-
-
-
-
-
 1
c
y
l
i
n
d
e
r 1  1
r
a
d
i
u
s
= 2
.0000
+
z
= 10
.000
-
z
=
-10
.000
c
e
n
t
e
r
l
i
n
e
i
```

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```
 2
c
u
b
o
i
d   2  1
+
x
= 3
.5464
-
x
=
-3
.5464
+
y
= 3
.5464
-
y
=
-3
.5464
+
z
= 12
.000
-
z
=
-12
.000

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```

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```

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```
                                10
x10
x2
a
r
r
a
y
d
i
m
e
n
s
i
o
n
s
e
a
r
c
h
-
c
h
a
n
g
e
i
n
x
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y

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b
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s
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g
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t
e
s
t
i
m
a
t
e
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f
t
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a
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a
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e
t
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i
s   -1.16433E-01
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t
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m
e
t
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y
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r
e
s
p
o
n
d
i
n
g
t
o
t
h
i
s
p
a
r
a
m
e
t
e
r
f
o
l
l
o
w
s
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m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
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```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
-
 1
c
y
l
i
n
d
e
r 1  1
r
a
d
i
u
s
= 2
.0000
+
z
= 10
.000
-
z
=
-10
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c
e
n
t
e
r
1
i
n
e
i
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   2  1
+
x
= 3
.5343
-
x
=
-3
.5343
+
y
= 3
.5343
-
y
=
-3
.5343
+
z
= 12
.000
-
z
=
-12
.000

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8.11.4 Array of Centered Uranium Slabs

Consider a 10 × 1 × 1 array of uranium metal slabs. The uranium slabs are 2 cm thick in the X dimension and 200 cm thick in the Y and Z dimensions. On each side of the uranium slab in the X dimension is 1 cm of H_2O, then 1 cm of Boral, then 1 cm of H_2O resulting in an initial center-to-center spacing of 8.0 cm. The slabs are 90% ^{235}U and 10% ^{238}U, the water is full density, and the Boral is 36.7% B_4C. The uranium slabs and their associated materials are defined to be Unit 1, and the 10 × 1 × 1 array is defined to be array 1. The problem searches for the slab center-to-center spacing that will produce a k_{eff} = 1.0 for the system, which is the default search value. Because this is a dimension search all search data must be specified. The +X and X search constants are specified as well as the CON and +CON search constraints. The search data is set up to alter the cylinder change the water slab thickness between the Boral plates from 0.8 cm to 10.0 cm thick during the search. The MORE search data CELL=1 ties the search data to the first unit cell thus ensuring they change in unison properly modifying the cross-section processing. The input data and the final search results for this problem follow:

```
=CSAS5S
10
x1
x1
A
R
R
A
Y
D
I
M
E
N
S
I
O
N
S
E
A
R
C
H
-
S
L
A
B

V7
-238

R
E
A
D
C
O
M
P
```

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```
U
R
A
N
I
U
M 1 1
.0   300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 1
.0   300
.0
E
N
D

B4
C     3 0
.367 300
.0
E
N
D

A
L      3 0
.633 300
.0
E
N
D

H2
O     4 1
.0   300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
```

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```
L
A
T
T
I
C
E
C
E
L
L
S
Y
M
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S
L
A
B
C
E
L
L
P
I
T
C
H
=8
.0 4
F
U
E
L
D
=2
.0 1

G
A
P
D
=6
.0 3
C
L
A
D
D
=4
.0 2
E
N
D

E
N
D
C
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L
L
D
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U
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D  1 1 1
.0
-1
.0  4
P100
.0

C
U
B
O
I
D  2 1 2
.0
-2
.0  4
P100
.0

C
U
B
O
I
D  3 1 3
.0
-3
.0  4
P100
.0

C
U
B
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I
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.0
-4
.0  4
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R
E
A
D
A
R
R
A
Y

A
R
A
=1
G
B
L
=1
N
U
X
=10
N
U
Y
=1
N
U
Z
=1
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y
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O
R
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A
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R
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N
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=1
R
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G
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=  1
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+00
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-  1
.79880
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s  4
k
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=  9
.99495
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-01
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s
s  4
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a
r
a
m
e
t
e
r
w
a
s   1.80331E-01

t
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q
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a
t
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d
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k
-
e
f
f
=
+1
.13914
E
+00
-9
.36766
E
-01
*
p
+9
.20374
E
-01
*
p
*
*2
-1
.09475
E
-01
*
p
*
*3


k
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f
f
e
c
t
i
v
e
=  9
.99495
E
-01
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o
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-  1
.65714
E
-03
t
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c
o
r
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m
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c
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d

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-
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u
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i
t      1
-
-
-
-
-
-
 1
c
u
b
o
i
d   1  1
+
x
= 1
.0000
-
x
=
-1
.0000
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00
 3
c
u
b
o
i
d   3  1
+
x
= 3
.0000
-
x
=
-3
.0000
+
y
= 100
.00
-
y
=
```

(continues on next page)

```
-100
.00
+
z
= 100
.00
-
```

(continued from previous page)

```
 4
c
u
b
o
i
d   4  1
+
x
= 4
.7213
-
x
=
-4
.7213
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00

*
*
*
```

(continued from previous page)

```
*
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*
```

(continued from previous page)

```
                                    10
x1
x1
a
r
r
a
y
d
i
m
e
n
s
i
o
n
s
e
a
r
c
h
-
s
l
a
b

*
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```

(continued from previous page)

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*
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(continued from previous page)

```
b
a
s
e
d
o
n
t
h
e
p
r
e
c
e
d
i
n
g
d
a
t
a
,
t
h
e
b
e
s
t
e
s
t
i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s    1.79511E-01
```

(continues on next page)

(continued from previous page)

```
t
h
e
g
e
o
m
e
t
r
y
c
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r
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s
p
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n
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g
t
o
t
h
i
s
p
a
r
a
m
e
t
e
r
f
o
l
l
o
w
s
:

m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
```

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(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
-
 1
c
u
b
o
i
d   1  1
+
x
= 1
.0000
-
x
=
-1
.0000
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   2  1
+
x
= 2
.0000
-
x
=
-2
.0000
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00
 3
c
u
b
o
i
d   3  1
+
x
= 3
.0000
-
x
=
-3
.0000
+
y
= 100
.00
-
y
=
```

(continues on next page)

```
-100
.00
+
z
= 100
.00
-
```

(continued from previous page)

```
 4
c
u
b
o
i
d   4  1
+
x
= 4
.7180
-
x
=
-4
.7180
+
y
= 100
.00
-
y
=
-100
.00
+
z
= 100
.00
-
z
=
-100
.00

*
*
*
```

(continued from previous page)

```
*
*
*
```

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8.11.5 Search on Multiple Units and Regions

Consider a problem having Units 1, 2, and 3. Unit 1 consists of three concentric spheres in a cuboid. Unit 2 consists of a single sphere in a cuboid, and Unit 3 contains three concentric cuboids. A search is to be made that changes the exterior dimensions of the three units, the inner sphere of Unit 1, and the sphere of Unit 2. The thicknesses of the outer spheres of Unit 1 are to be maintained, and the two inner cuboids of Unit 3 are to remain unchanged. The search data and results for this problem are the following:

```
=CSAS5S

D
E
M
O
N
S
T
R
A
T
I
O
N
O
F
C
R
I
T
I
C
A
L
D
I
M
E
N
S
I
O
N
S
E
A
R
C
H

V7
-252

R
E
A
D
O
M
P
```

(continues on next page)

(continued from previous page)

```
U
R
A
N
I
U
M  1 0
.985 293  92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2
E
N
D

P
L
E
X
I
G
L
A
S  2
E
N
D

S
S304    3
E
N
D

E
N
D
C
O
M
P

R
E
A
D
P
A
R
A
M
E
T
E
R
S
G
E
N
=203
N
P
```

(continues on next page)

(continued from previous page)

```
E
N
D
P
A
R
A
M
E
T
E
R
S

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

S
P
H
E
R
E 1 1 3
.0

S
P
H
E
R
E 0 1 3
.25

S
P
H
E
R
E 2 1 3
.5

C
U
B
E 0 1 2
P5
.0
```

(continues on next page)

(continued from previous page)

```
U
N
I
T 2

S
P
H
E
R
E 1 1 3
.0

C
U
B
E   0 1 2
P5
.0

U
N
I
T 3

C
U
B
E   0 1 2
P4
.9

C
U
B
E   3 1 2
P5
.0

C
U
B
E   0 1 2
P5
.0

E
N
D
G
E
O
M
E
T
R
Y
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y
A
R
A
=1
N
U
X
=3
N
U
Y
=3
N
U
Z
=3
F
I
L
L
1 3 2 3 2 3 2 3 1
3 2 3 1 3 2 3 1 3
2 3 1 3 1 3 1 3 2

E
N
D
F
I
L
L
E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
S
E
A
R
C
H
C
R
I
T
I
C
A
L
D
I
M
E
N
S
I
O
N

K
E
F
=1
.000
E
P
S
=0
.005
M
O
R
E

A
L
T
E
R
U
N
I
T
=1
R
E
G
=1
A
L
L
=1
.0
```

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```
A
L
T
E
R
U
N
I
T
=1
R
E
G
=4
A
L
L
=1
.0

A
L
T
E
R
U
N
I
T
=2
R
E
G
=1
T
O 2
A
L
L
=1
.0

A
L
T
E
R
U
N
I
T
=3
R
E
G
=3
```

(continues on next page)

```
A
L
L
=1
.0
```

(continued from previous page)

```
M
A
I
N
T
A
I
N
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N
I
T
=1
R
E
G
=2
T
O 3
A
L
L
=1
.0

+
C
O
N
=2
.0
-
C
O
N
=
-0
.5

E
N
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S
E
A
R
C
H

E
N
D
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t
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e
t
e
r
w
a
s  0.00000E+00

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v
d
a
t
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b
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i
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t  95
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a
s
s  2
k
e
f
f
=  1
.07404
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.44587
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-03
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s  2.00000E+00

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s
s  4
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.94811
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.34462
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s
e
a
r
c
h
p
a
s
s  5
k
e
f
f
=  9
.99482
E
-01
+
o
r
-  1
.35858
E
-03
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```
t
h
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p
a
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a
m
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t
e
r
w
a
s  1.73183E+00

s
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c
h
d
e
m
o
n
s
t
r
a
t
i
o
n
o
f
c
r
i
t
i
c
a
l
d
i
m
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r
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c
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w
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s
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c
h
i
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v
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d
o
n
p
a
s
s  5
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s   1.73183E+00

t
h
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q
u
a
t
i
o
n
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s
e
d
i
n
t
h
```

(continues on next page)

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```
k
-
e
f
f
=
+4
.05037
E
-01
-7
.56139
E
-02
*
p
+4
.77691
E
-01
*
p
*
*2
-1
.36173
E
-01
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  9
.99482
E
-01
+
o
r
-  1
.35858
E
-03
t
h
e
c
o
r
```

(continues on next page)

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```
m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
r
y
d
e
s
c
r
i
p
t
i
o
n
f
o
r
t
h
o
s
e
u
n
i
t
s
u
t
i
l
i
z
e
d
i
n
t
h
i
s
p
r
o
b
l
e
m
```

(continues on next page)

(continued from previous page)

```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
=  8
.1955
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
```

(continues on next page)

(continued from previous page)

```
 2
s
p
h
e
r
e   0  1
r
a
d
i
u
s
=  8
.4455
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
,  0
.0000
,  0
.0000
)
.
 3
s
p
h
e
r
e   2  1
r
a
d
i
u
s
=  8
.6955
t
h
e
c
e
n
```

(continues on next page)

(continued from previous page)

```
 4
c
u
b
o
i
d   0  1
+
x
=  13
.659
-
x
=
-13
.659
+
y
=  13
.659
-
y
=
-13
.659
+
z
=  13
.659
-
z
=
-13
.659


-
-
-
-
-
-
u
n
i
t     2
-
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
=  8
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   0  1
+
x
=  13
.65
-
x
=
-13
.659
+
y
=  13
.659
-
y
=
-13
.659
+
z
=  13
.659
-
z
=
-13
.659


-
-
-
-
-
u
n
i
t     3
-
-
-
-
-
 1
c
u
b
o
i
d   0  1
```

(continues on next page)

```
+
x
=  4
.9000
-
x
=
```

(continued from previous page)

```
 2
c
u
b
o
i
d   3  1
+
x
=  5
.0000
-
x
=
-5
.0000
+
y
=  5
.0000
-
y
=
-5
.0000
+
z
=  5
.0000
-
z
=
-5
.0000
 3
c
u
b
o
i
d   0  1
+
x
=  13
.659
-
x
=
-13
.659
+
y
=  13
.659
-
y
=
```

(continues on next page)

```
-13
.659
+
z
=  13
.659
-
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
s
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a
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c
h
d
e
m
o
n
s
t
r
a
t
i
o
n
o
f
c
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t
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c
a
l
d
i
m
e
n
s
i
o
n
s
e
a
r
c
h

*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
b
a
s
e
d
o
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t
h
e
p
r
e
c
e
d
i
n
g
d
a
t
a
,
t
h
e
b
e
s
t
e
s
t
i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s    1.73328E+00
```

(continues on next page)

(continued from previous page)

```
t
h
e
g
e
o
m
e
t
r
y
c
o
r
r
e
s
p
o
n
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i
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g
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o
t
h
i
s
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a
r
a
m
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t
e
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o
l
l
o
w
s
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m
e
d
i
a
b
i
a
s
g
e
o
m
e
t
```

(continues on next page)

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```
r
e
g
i
o
n
n
u
m
i
d

-
-
-
-
-
-
u
n
i
t      1
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
=  8
.1998
t
h
e
c
e
n
t
e
r
i
s
l
o
c
a
t
e
d
a
t
(  0
.0000
```

(continues on next page)

(continued from previous page)

```
 2
s
p
h
e
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e   0  1
r
a
d
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u
s
=  8
.4498
t
h
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c
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i
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a
t
(  0
.0000
,  0
.0000
,  0
.0000
)
.
 3
s
p
h
e
r
e   2  1
r
a
d
i
u
s
=  8
.6998
t
h
e
c
e
n
```

(continues on next page)

(continued from previous page)

```
 4
c
u
b
o
i
d   0  1
+
x
=  13
.666
-
x
=
-13
.666
+
y
=  13
.666
-
y
=
-13
.666
+
z
=  13
.666
-
z
=
-13
.666

-
-
-
-
-
u
n
i
t     2
-
-
-
-
-
 1
s
p
h
e
r
e   1  1
r
a
d
i
u
s
=  8
.1998
```

(continues on next page)

(continued from previous page)

```
 2
c
u
b
o
i
d   0  1
+
x
=  13
.666
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x
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-13
.666
+
y
=  13
.666
-
y
=
-13
.666
+
z
=  13
.666
-
z
=
-13
.666


-
-
-
-
-
u
n
i
t     3
-
-
-
-
-
 1
c
u
b
o
i
d   0  1
```

(continues on next page)

```
+
x
=  4
.9000
-
x
=
```

(continued from previous page)

```
 2
c
u
b
o
i
d   3  1
+
x
=  5
.0000
-
x
=
-5
.0000
+
y
=  5
.0000
-
y
=
-5
.0000
+
z
=  5
.0000
-
z
=
-5
.0000
 3
c
u
b
o
i
d   0  1
+
x
=  13
.666
-
x
=
-13
.666
+
y
=  13
.666
-
y
=
```

(continues on next page)

```
-13
.666
+
z
=  13
.666
-
```

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```
*
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8.11.6 UO_2F_2 Solution Tank — Critical Search on Chord Length

Consider a large spherical tank partially filled with UO_2F_2 solution. The tank has a radius of 34.6 cm and is initially filled with solution to a height of 10.0 cm above the midpoint. The tank is composed of a 0.759-cm-thick Al shell. The UO_2F_2 solution is composed of three standard compositions: UO_2F_2, HF acid, and H_2O. The code combines these using a set algorithm. This may or may not produce a solution at the desired density. If the density of the solution is known it should be entered. Also, extra acid can be added to the solution by specifying a non-zero acid molarity.

A critical dimension search is performed on the length of the chord yielding system k_{eff} = 0.98. In the MORE search data, UNIT=1 REG=1 CHORD=1 specifies that the chord length of region 1 in Unit 1 is to be altered with the limits defined by the search constraints. The minimum search constraint is set so region 1 consists of the part of the sphere below an X-Y plane 10.0 cm below the sphere's midpoint. The maximum search constraint is set so region 1 consists of almost the entire sphere.

The constraints are calculated as follows:

$$D_i = (Radius_i + Chord_i) / (2*Radius_i) = (34.6 + 10.0) / 2*34.6) = 0.6445$$

$$D_{min} = (Radius_{min} + Chord_{min}) / (2*Radius_{min}) = (34.6 + 10.0) / 2*34.6) = 0.3555$$

$$D_{max} = (Radius_{max} + Chord_{max}) / (2*Radius_{max}) = (34.6 + 34.6) / 2*34.6) = 1.0$$

The maximum constraint is calculated according to:

$$+CON = [(D_{max} / D_i) 1.0] / CHORD = [(1.0 / 0.6445) 1.0] / 1.0 = 0.5515$$

The minimum constraint is calculated according to:

$$CON = [(D_{min} / D_i) 1.0] / CHORD = [(0.3555 / 0.6445) 1.0] / 1.0 = 0.4484$$

The search data and final search results for this problem follow:

```
=csas5s

s
a
m
p
l
e
p
r
o
b
l
e
m 6
s
o
l
n
t
a
n
k
-
c
```

(continues on next page)

```
r
i
t
.
d
i
m
```

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```
v7
-238
read
 comp

s
o
l
n
u
o2
f2  1 500 0 1 300
.0 92235 4
.89 92238 95
.09 92234 0
.02 end

a
l          2 1
.0 300
.0 end
end
 comp

s
a
m
p
l
e
p
r
o
b
l
e
m 6
s
o
l
n
t
a
n
k
-
c
r
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i
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read
 geom

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n
i
t 1

h
e
m
i
s
p
h
e
-
z  1 1 34
.6
c
h
o
r
d 10
.

s
p
h
e
r
e      0 1 34
.6

s
p
h
e
r
e      2 1 34
.759
end
 geom
end
 data

R
E
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S
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-0
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the parameter was  2.37245E-01

solution tank-critical dimensions search on chord length
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.82174
E
-01
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*2
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.30631
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t      1
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h
e
m
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e 1 1
r
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2
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a
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.0000
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, 0
.0000
)
.
3
s
p
h
e
r
e      2 1
r
a
d
i
u
s
= 34
.759
t
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e
c
e
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8.12 Optimum concentration search

An optimum concentration search alters the concentration of the specified standard composition in the specified mixture to determine the highest value of k_{eff}. The limits for an optimum concentration search are governed by the values entered for the parameter constraints. An optimum concentration search is activated by entering "OPTIMUM CONCENTRATION" in the search data. No defaulted search data are in a concentration search. The user must specify the material and standard composition name to be changed and the manner in which they will be changed.

A concentration search is performed by altering the atom densities of the specified standard compositions in the specified materials. The ratio of how the standard compositions change relative to each other is controlled using FACTOR. If a material and standard composition is not listed in the search data it remains unchanged. The concentration search can vary from zero to some upper limit. The code will prevent the concentration from falling below zero, but the user is responsible for setting constraints that prevent the concentration from exceeding reasonable values. In most cases the theoretical density is a reasonable upper limit.

8.12.1 Array of Spheres in H_2O — Search on H_2O Density

Consider a 10 × 10 × 10 array of uranium spheres arranged in an array having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the 10 × 10 × 10 array is defined to be array 1. The spheres are initially moderated by ½ density water.

An optimum concentration search is performed on the water yielding the maximum system k_{eff} for various densities of water. In the MORE search data, MIX=2 and SCNAME=H2O specify that the water component of mixture 2 is to be altered during the search. The maximum allowed density is full density water. The minimum allowed density is 0.05 density water.

The maximum constraint is calculated according to:

$$+\text{CON} = \frac{\left(\frac{\text{D}_{max}}{\text{D}_{initial}} - 1\right)}{\text{FACTOR}} \qquad +\text{CON} = \frac{\left(\frac{1.0}{0.5} - 1\right)}{1} = \frac{1}{0}$$

The minimum constraint is calculated according to:

$$-\text{CON} = \frac{\left(\frac{\text{D}_{min}}{\text{D}_{initial}} - 1\right)}{\text{FACTOR}} \qquad -\text{CON} = \frac{\left(\frac{0.05}{0.5} - 1\right)}{1} = -0.9$$

The search data and final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
-
C
O
N
C
E
N
T
R
A
T
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```
V7
-238

R
E
A
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C
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U
R
A
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U
M 1 1
.0 300
.0 92235 90
.0 92238 10
.0
E
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H2
O     2 0
.5 300
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P4
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-01
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.39277
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-02  9
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-01  92235  235
.0441   92
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/89
 1092238  4
.81921
E
-03  1
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-01  92238  238
.0510   92
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.48291
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.11926
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.0077
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/1002
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/92
 2008016 1
.74146
E
-02  8
.88073
E
-01  8016  15
.9904    8
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```
mixingtable

numberofscatteringangles= 2

crosssectionmessage
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/89
 1092238  4
.81921
E
-03 1
.00000
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-01  92238  238
.0510  92
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 2001001  3
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-02  1
.11927
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-01   1001    1
.0077
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e
r 1301
/1002
m
o
d1   11
/23
/92
 2008016  1
.76029
E
-02  8
.88073
E
-01   8016   15
.9904   8
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8.12.2 Array of Cylinders in H_2O — Search on H_2O Density

This problem contains search data for an optimum concentration search. The problem consists of a 10 × 10 × 1 array of uranium cylinders surrounded initially by 0.5 gm/cc density water. The cylinders are 90% ^{235}U and 10% ^{238}U and have a radius of 2.0 cm and a length of 200 cm. The cylinders are originally centered on an 8.0 cm X and Y pitch with interstitial low density (0.5 gm/cc) water. The problem searches for the H_2O density that will produce the maximum system k_{eff}. In the MORE search data, MIX=2 and SCNAME=H2O specify that the water component of mixture 2 is to be altered during the search. The maximum allowed density is full density water. The minimum allowed density is 0.05 density water.

The maximum constraint is calculated according to:

$$+\text{CON} = \frac{\left(\frac{\text{D}_{max}}{\text{D}_{initial}} - 1\right)}{\text{FACTOR}} \qquad +\text{CON} = \frac{\left(\frac{1.0}{0.5} - 1\right)}{1} = -1.0$$

The minimum constraint is calculated according to:

$$-\text{CON} = \frac{\left(\frac{\text{D}_{min}}{\text{D}_{initial}} - 1\right)}{\text{FACTOR}} \qquad -\text{CON} = \frac{\left(\frac{0.05}{0.5} - 1\right)}{1} = -0.9$$

The search data and final search results for this problem follow:

```
=CSAS5S
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x10
x1
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R
A
Y
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R
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C
H
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E
H2
O
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V7
-238

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.0 300
.0 92235 90
.0 92238 10
.0
E
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H2
O     2 0
.5 300
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.63481
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p
-2
.85686
E
-01
*
p
*
*2
+1
.05562
E
-01
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  1
.63831
E
+00
+
o
r
-  1
.43843
E
-03
t
h
e
c
o
r
```

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(continued from previous page)

```
                                10
x10
x10
a
r
r
a
y
c
o
n
c
e
n
t
r
a
t
i
o
n
s
e
a
r
c
h
-
c
h
a
n
g
e
h2
o

m
i
x
i
n
g
t
a
b
l
e

n
u
m
b
e
r
o
f
s
c
a
t
t
e
r
```

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```
c
r
o
s
s
s
e
c
t
i
o
n
m
e
s
s
a
g
e
t
h
r
e
s
h
o
l
d =5.7E-02

m
i
x
t
u
r
e
=     1
d
e
n
s
i
t
y
(
g
/
c
c
)
=  19
.050

n
u
c
l
i
d
e
a
t
```

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```
 1092235  4
.39277
E
-02  9
.00000
E
-01  92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
m
o
d3 02
/28
/89
 1092238  4
.81921
E
-03  1
.00000
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
U
N77
E
.
P
E
N
N
I
N
G
T
O
N
```

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m
i
x
t
u
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e
=      2
d
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n
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i
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y
(
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/
c
c
)
= 0
.56371

n
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o
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d
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n
s
.
w
g
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.
f
r
a
c
.
z
a
a
w
t
```

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```
n
u
c
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i
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```

(continued from previous page)

```
 2001001  3
.77076
E
-02  1
.11926
E
-01  1001   1
.0077
h
y
d
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o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1   11
/23
/92
 2008016  1
.88538
E
-02  8
.88073
E
-01  8016  15
.9904  8
O 16
f
r
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m
v
e
r
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i
o
n 6
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l
u
a
t
i
o
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c
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i
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d
a
t
a
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t
h
e
b
e
s
t
e
s
t
i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s    1.16606E-01
```

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(continued from previous page)

```
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i
x
i
n
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t
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b
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e
c
o
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s
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o
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i
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t
h
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a
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a
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t
e
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f
o
l
l
o
w
s
:
                                10
x10
x10
a
r
r
a
y
c
o
n
c
e
```

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```
mixingtable

numberofscatteringangles= 2

crosssectionmessage
```

(continues on next page)

```
getnres
```

(continued from previous page)

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m
i
x
t
u
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=     1
d
e
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y
(
g
/
c
c
)
=  19
.050

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n
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```

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```
 1092235  4
.39277
E
-02 9
.00000
E
-01  92235  235
.0441  92
u 235
b
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e
v
a
l
a
p
r77
m
.
r
.
b
h
a
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m
o
d3 02
/28
/89
 1092238  4
.81921
E
-03 1
.00000
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
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J
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N77
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c
)
= 0
.55728

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```
 2001001  3
.72774
E
-02  1
.11927
E
-01  1001   1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1 11
/23
/92
 2008016  1
.86387
E
-02  8
.88074
E
-01  8016  15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
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o
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8.12.3 Cell-Weighted Array of Uranium Cylinders in H_2O — Search on H_2O Density

This problem contains search data for an optimum concentration search. The problem consists of a single material representing a 10 × 10 × 1 array of uranium cylinders surrounded initially by 0.5 gm/cc density water. The cylinders are 90% ^{235}U and 10% ^{238}U and have a radius of 2.0 cm and a length of 200 cm. The cylinders are originally centered on an 8.0 cm X and Y-pitch with interstitial low density (0.5 gm/cc) water. The keyword CELL=100 in the unit cell data indicates this will be a cell-weighted problem with mixture 100 representing the array of uranium rods in water. The problem searches for the H_2O density that will produce the maximum system k_{eff}. In the MORE search data, MIX=2 and SCNAME=H_2O specify that the water component of mixture 2 is to be altered during the search. On each pass the water density is altered, XSDRNPM is run to produce a new mixture 100, and mixture 100 is used in KENO V.a to calculate a new system k_{eff}. The cylinder and cuboid in unit 1 and the array contained in the above problem are replaced by a cuboid of the same size as the array containing mixture 100. The maximum allowed density is full density water. The minimum allowed density is 0.05 density water.

The maximum constraint is calculated according to:

$$+\text{CON} = \frac{\left(\frac{\text{D}_{max}}{\text{D}_{initial}} - 1\right)}{\text{FACTOR}} \qquad +\text{CON} = \frac{\left(\frac{1.0}{0.5} - 1\right)}{1} = -1.0$$

The minimum constraint is calculated according to:

$$-\text{CON} = \frac{\left(\frac{\text{D}_{min}}{\text{D}_{initial}} - 1\right)}{\text{FACTOR}} \qquad -\text{CON} = \frac{\left(\frac{0.05}{0.5} - 1\right)}{1} = -0.9$$

The search data and final search results for this problem follow:

```
=CSAS5S
10
x10
x1
A
R
R
A
Y
C
O
N
C
E
N
T
R
A
T
I
O
N
S
E
A
R
C
H
```

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```
-
C
H
A
N
G
E
```

(continued from previous page)

```
V7
-238

R
E
A
D
C
O
M
P

U
R
A
N
I
U
M 1 1
.0 300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.5 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A
```

(continues on next page)

```
L
A
T
I
I
C
E
```

(continued from previous page)

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E
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D
C
E
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L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

C
U
B
O
I
D  100 1 4
p40
.0  2
p100
.0

E
N
D
G
E
O
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E
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D
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O
N
M
O
R
E

A
L
T
E
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X
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C
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A
M
E
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H2
O
F
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C
T
O
R
=1
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C
O
N
=
-0
.9
+
C
O
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.0

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H

E
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i
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t
e
r
v
a
l
s
*
*
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*
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.67697
E
-03
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s -9.00000E-01

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c
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a
s
s  3
k
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=  1
.51930
E
+00
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.21366
E
-03
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s  1.00000E+00

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```
        20
mesh interval sin zone  2

*****modified keno v.data has been rewritten
```

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on unit 25
```

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s  4
k
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=  1
.61577
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.47397
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-03
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a
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t
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h
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s
b
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e
n
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w
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i
t
t
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n
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n
u
n
i
t  25
```

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s
e
a
r
c
h
p
a
s
s  5
k
e
f
f
=  1
.64316
E
+00
+
o
r
-  1
.70752
E
-03
*
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```
t
h
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m
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t
e
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w
a
s  1.35197E-01
                                10
x10
x10
a
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r
a
y
c
o
n
c
e
n
t
r
a
t
i
o
n
s
e
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c
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h2
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s   1.35197E-01

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```
k
-
e
f
f
=
+1
.63882
E
+00
+6
.77742
E
-02
*
p
-2
.75913
E
-01
*
p
*
*2
+8
.93705
E
-02
*
p
*
*3


k
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(continues on next page)

(continued from previous page)

```
                                        10
x10
x10
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r
r
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c
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t
r
a
t
i
o
n
s
e
a
r
c
h
-
c
h
a
n
g
e
h2
o

m
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c
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s
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g
e
t
h
r
e
s
h
o
l
d =5.7E-02

m
i
x
t
u
r
e
=     1
d
e
n
s
i
t
y
(
g
/
c
c
)
=  19
.050

n
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c
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(continues on next page)

(continued from previous page)

```
 1092235  4
.39277
E
-02  9
.00000
E
-01  92235  235
.0441  92
u 235
b
n
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.
b
h
a
t
m
o
d3 02
/28
/89
 1092238  4
.81921
E
-03  1
.00000
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
U
N77
E
.
P
E
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N
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O
N
```

(continues on next page)

(continued from previous page)

```
m
i
x
t
u
r
e
=      2
d
e
n
s
i
t
y
(
g
/
c
c
)
= 0
.56656

n
u
c
l
i
d
e
a
t
o
m
-
d
e
n
s
.
w
g
t
.
f
r
a
c
.
z
a
a
w
t
```

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```
n
u
c
l
i
d
e
```

(continued from previous page)

```
 2001001  3
.78981
E
-02  1
.11926
E
-01  1001   1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1   11
/23
/92
 2008016  1
.89490
E
-02  8
.88073
E
-01  8016  15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
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n 6
e
v
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l
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a
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m
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x
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e
=   100
d
e
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c
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=  0
.0000

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c
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z
a
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w
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c
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```
 2001001  0
.00000
E
+00  0
.00000
E
+00   1001    1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1   11
/23
/92
 2008016  0
.00000
E
+00  0
.00000
E
+00   8016   15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
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o
n
```

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(continued from previous page)

```
 1092235  0
.00000
E
+00  0
.00000
E
+00  92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
m
o
d3 02
/28
/89
 1092238  0
.00000
E
+00  0
.00000
E
+00  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
U
N77
E
.
P
E
N
N
I
N
G
T
O
N
```

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```
b
a
s
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d
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i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s    1.31179E-01
```

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```
t
h
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m
i
x
i
n
g
t
a
b
l
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c
o
r
r
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s
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o
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t
h
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a
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l
o
w
s
:
                                10
x10
x10
a
r
r
a
y
c
o
n
c
```

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```
mixingtable
numberofscatteringangles= 2
crosssectionmessageth
resh
```

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m
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=     1
d
e
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i
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g
/
c
c
)
=  19
.050

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d
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a
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m
-
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n
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g
t
.
f
r
a
c
.
z
a
a
w
t
n
u
c
l
i
d
e
```

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(continued from previous page)

```
 1092235  4
.39277
E
-02  9
.00000
E
-01  92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
m
o
d3 02
/28
/89
 1092238  4
.81921
E
-03  1
.00000
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
U
N77
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P
E
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N
I
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T
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```

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=      2
d
e
n
s
i
t
y
(
g
/
c
c
)
= 0
.56455

n
u
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t
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d
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n
s
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z
a
a
w
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```

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```
n
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d
e
```

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```
 2001001  3
.77639
E
-02  1
.11927
E
-01  1001   1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1   11
/23
/92
 2008016  1
.88820
E
-02  8
.88074
E
-01  8016  15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
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u
a
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i
o
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```

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```
m
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c
)
=  0
.0000

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```
 2001001  0
.00000
E
+00  0
.00000
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+00   1001    1
.0077
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w
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t
e
r 1301
/1002
m
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d 11
/23
/92
 2008016  0
.00000
E
+00  0
.00000
E
+00   8016   15
.9904  8
O 16
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```
 1092235  0
.00000
E
+00  0
.00000
E
+00  92235  235
.0441  92
u 235
b
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v
a
l
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p
r77
m
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r
.
b
h
a
t
m
o
d3 02
/28
/89
 1092238  0
.00000
E
+00  0
.00000
E
+00  92238  238
.0510  92
U 238
A
N
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+
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V
A
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```

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8.13 Minimum concentration search

A minimum concentration search searches for the standard composition density that yields the lowest value of k_{eff}. A minimum concentration search is activated by entering "MINIMUM CONCENTRATION" in the search data. There are no defaulted search data in a concentration search. The user must specify the material and standard composition name to be changed and the manner in which they will be changed as described in the auxiliary search commands.

A concentration search is performed by altering the atom densities of the specified standard compositions in the specified materials. The ratio of how the standard compositions change relative to each other is controlled using FACTOR. If a material and standard composition is not listed in the search data it remains unchanged. The concentration search can vary from zero to some upper limit. The code will prevent the concentration from falling below zero, but the user is responsible for setting constraints that prevent the concentration from exceeding reasonable values. In most cases the theoretical density is a reasonable upper limit.

8.13.1 Infinite Array of Fuel Bundles Separated by Flux Traps — Search on H_2O Density in Trap

The fuel bundles in this problem represent 17 × 17 PWR fuel assemblies. The fuel pins are smeared together, making a mixture 100. The fuel pins consist of 2.35 wt % ^{235}U having a diameter of 0.823 cm, zirconium cladding having an outer diameter of 0.9627 cm, and a pitch of 1.275 cm. The fuel bundle is represented as a 10.8375 cm × 10.8375 cm × 366 cm cuboid of mixture 100 surrounded by Boral and then water. The Boral has a density of 2.65 g/cm^3 and is composed of 35.17 wt % B_4C and 64.83 wt % Al. The fuel bundles are at a fixed pitch of 13.0 cm. This is the same problem as described for a minimum dimension search above with the water component of the trap size optimized, thus producing a minimum system k_{eff}. The input data and the final search results for this problem follow:

```
=csas5s

a
r
r
a
y
o
f
f
u
e
l
b
u
n
d
l
e
s
w
i
t
h
f
l
u
x
t
r
a
p
```

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```
v7
-238
read
 comp

u
o2    1
.84 300
.  92235 2
.35 92238 97
.65 end

z
r     2 1 end

h2
o    3 1 end

b4
c    4
d
e
n
=2
.65 0
.3517 end

a
l     4
d
e
n
=2
.65 0
.6483 end

h2
o    5 0
.5 end
end
 comp
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
```

(continues on next page)

```
q
u
a
r
e
p
i
```

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```
end
 celldata
read
 param
 far
=yes
 gen
=
2
0
3
 npg
=
1
0
0
0
 end
 param
read
 geom

c
u
b
o
i
d 100 1 4
p10
.8375 2
p183
.0

c
u
b
o
i
d   4 1 4
p11
.0    2
p183
.0

c
u
b
o
i
d   5 1 4
p13
.0    2
p183
.0
end
 geom
read
```

(continues on next page)

```
 bounds
 xfc
=mirror
 yfc
=mirror
 end
 bounds
```

(continued from previous page)

```
end
 data
read
 search

 minimum
 concentration

 more

a
l
t
e
r
m
i
x
=5
s
c
n
a
m
e
=
h2
o
f
a
c
t
o
r
=1
.0

-
c
o
n
=
-0
.9
+
c
o
n
=1
.0
end
 search
end
```

```
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```

(continues on next page)

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```

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```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

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*
*
*
x
s
d
r
n
p
m
m
e
s
h
i
n
t
e
r
v
a
l
s
*
*
*
*
     4
m
e
s
h
i
n
t
e
r
v
a
l
s
i
n
z
o
n
```

(continues on next page)

(continued from previous page)

```
     4
m
e
s
h
i
n
t
e
r
v
a
l
s
i
n
z
o
n
e  2
    14
m
e
s
h
i
n
t
e
r
v
a
l
s
i
n
z
o
n
e  3

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d
i
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i
e
d
k
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v
d
a
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a
h
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s
e
a
r
c
h
p
a
s
s  2
k
e
f
f
=  8
.62695
E
-01
+
o
r
-  1
.43366
E
-03
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t
h
e
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a
r
a
m
e
t
e
r
w
a
s -9.00000E-01

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x
s
d
r
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m
m
e
s
h
i
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e
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v
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l
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     4
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e
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```

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```
     4
m
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e  3

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v
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a
h
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s
e
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r
c
h
p
a
s
s  3
k
e
f
f
=  7
.04284
E
-01
+
o
r
-  1
.44875
E
-03
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t
h
e
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e
t
e
r
w
a
s  1.00000E+00

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x
s
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n
z
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i
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e  3

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k
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o
v
d
a
t
a
h
```

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*
s
e
a
r
c
h
p
a
s
s  4
k
e
f
f
=  7
.36291
E
-01
+
o
r
-  1
.54213
E
-03
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t
h
e
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a
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t
e
r
w
a
s  5.00000E-01

a
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r
a
y
o
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f
u
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l
b
u
n
d
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s
w
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h
f
l
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x
t
r
a
p

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```
c
o
n
v
e
r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  3
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s   1.00000E+00

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

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```
k
-
e
f
f
=
+7
.70310
E
-01
-7
.54970
E
-02
*
p
+2
.03650
E
-02
*
p
*
*2
-1
.08939
E
-02
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  7
.04284
E
-01
+
o
r
-  1
.44875
E
-03
t
h
e
c
o
r
```

(continues on next page)

(continued from previous page)

```
a
r
r
a
y
o
f
f
u
e
l
b
u
n
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l
e
s
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i
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h
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l
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x
t
r
a
p

m
i
x
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r
i
n
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a
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```
c
r
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s
s
e
c
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i
o
n
m
e
s
s
a
g
e
t
h
r
e
s
h
o
l
d =5.7E-02

m
i
x
t
u
r
e
=     1
d
e
n
s
i
t
y
(
g
/
c
c
)
=  9
.2064

n
u
c
l
i
d
e
a
t
```

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(continued from previous page)

```
1008016  4
.10743
E
-02  1
.18465
E
-01   8016   15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
o
n
1092235  4
.88650
E
-04  2
.07161
E
-02  92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
m
o
d3 02
/26
/89
```

(continues on next page)

(continued from previous page)

```
1092238  2
.00485
E
-02  8
.60819
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
U
N77
E
.
P
E
N
N
I
N
G
T
O
N
M
O
D3 02
/13
/92


m
i
x
t
u
r
e
=     2
d
e
n
s
i
t
y
(
g
/
c
c
)
=     8
.4900
```

(continues on next page)

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```
n
u
c
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e
2040000  4
.28457
E
-02  1
.00000
E
+00  40000   91
.2196  40
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3001001  6
.67692
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-02  1
.11927
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-01   1001    1
.0077
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r 1301
/1002
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o
d1 11
/23
/92
3008016  3
.33846
E
-02  8
.88074
E
-01   8016   15
.9904   8
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4005010  8
.08716
E
-03  5
.07413
E
-02   5010  10
.0130  5
b 100
l
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c76
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d1 12
/11
/92
f
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a
s
4005011  3
.25519
E
-02  2
.24568
E
-01   5011  11
.0096  5
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e
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```
4006012  1
.01598
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-02  7
.63956
E
-02   6000  12
.0001  6
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/92
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4013027  3
.83444
E
-02  6
.48295
E
-01  13027  26
.9818   13
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-02  1
.11927
E
-01   1001   1
.0077
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/23
/92
5008016  3
.33846
E
-02  8
.88074
E
-01   8016  15
.9904   8
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```
3001001  0
.00000
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+00  0
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+00   1001    1
.0077
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3008016  0
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+00   8016   15
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1008016  0
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2040000  0
.00000
E
+00  0
.00000
E
+00  40000   91
.2196  40
z
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d2 01
```

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1092235  0
.00000
E
+00  0
.00000
E
+00  92235  235
.0441  92
u 235
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e
v
a
l
a
p
r77
m
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r
.
b
h
a
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m
o
d3 02
/28
/89
1092238  0
.00000
E
+00  0
.00000
E
+00  92238  238
.0510  92
U 238
A
N
L
+
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V
A
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N77
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8.14 Critical concentration search

A critical concentration search alters the concentration of the specified standard composition in the specified mixture to obtain a specified value of k_{eff}. A critical concentration search is activated by entering "CRITICAL CONCENTRATION" in the search data. There are no defaulted search data in a critical concentration search except for the value of k_{eff}. If something other than k_{eff} = 1.0 is desired the user must specify KEF=**, where ** is the desired value of k_{eff}. The remaining data is entered after the keyword MORE in the search data block. The user must specify the material and standard composition name to be changed and the manner in which they will be changed as described in the auxiliary search commands.

A concentration search is performed by altering the atom densities of the specified standard compositions in the specified materials. The ratio of how the standard compositions change relative to each other is controlled using FACTOR. If a material and standard composition is not listed in the search data it remains unchanged. The concentration search can vary from zero to some upper limit. The code will prevent the concentration from falling below zero, but the user is responsible for setting constraints that prevent the concentration from exceeding reasonable values. In most cases the theoretical density is a reasonable upper limit.

8.14.1 Array of Spheres in H_2O — Search on H_2O Density

Consider a 10 × 10 × 10 array of uranium spheres arranged in an array having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the 10 × 10 × 10 array is defined to be array 1.0 cm. The spheres are initially moderated by ½ density water.

A critical concentration search is performed on the water yielding system k_{eff} = 1.0 for various densities of water. In the MORE search data, MIX=2 and SCNAME=H2O specify that the water component of mixture 2 is to be altered during the search from an initial density of 0.5 gm/cc. The maximum allowed density is full density water (1.0 gm/cc). The minimum allowed water density is 0.0005 gm/cc.

The maximum constraint is calculated according to:

+CON= (1.0/0.5 1)/1.0 = 1.0

The minimum constraint is calculated according to:

CON= (0.0005/0.5 1)/1.0 = 0.999

The search data and final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
-
C
O
N
C
```

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```
E
N
T
R
A
T
I
```

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```
V7
-238

R
E
A
D
C
O
M
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U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.5  300
.0
E
N
D

E
N
D
C
O
M
P

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L
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T 1

S
P
H
E
R
E  1 1 2
.0

C
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B
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D  2 1 6
P4
.0

E
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.90957
E
-01
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.41575
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+00
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p
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-1
.11098
E
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s
h
o
l
d =5.7E-02

m
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c
)
=  19
.050

n
u
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l
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e
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(continues on next page)

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1092235  4
.39277
E
-02  9
.00000
E
-01  92235  235
.0441  92
u 235
b
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e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
m
o
d3 02
/28
/89
1092238  4
.81921
E
-03  1
.00000
E
-01  92238  238
.0510  92
U 238
A
N
L
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m
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t
y
(
g
/
c
c
)
= 0
.23534

n
u
c
l
i
d
e
a
t
o
m
-
d
e
n
s
.
w
g
t
.
f
r
a
c
.
z
a
a
w
t
n
u
c
l
i
d
e
```

(continues on next page)

(continued from previous page)

```
2001001  1
.57425
E
-02  1
.11926
E
-01  1001    1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1   11
/23
/92
2008016  7
.87126
E
-03  8
.88074
E
-01  8016   15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
o
n
```

(continues on next page)

(continued from previous page)

```
b
a
s
e
d
o
n
t
h
e
p
r
e
c
e
d
i
n
g
d
a
t
a
,
t
h
e
b
e
s
t
e
s
t
i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s   -5.28963E-01
```

(continues on next page)

(continued from previous page)

```
t
h
e
m
i
x
i
n
g
t
a
b
l
e
c
o
r
r
e
s
p
o
n
d
i
n
g
t
o
t
h
i
s
p
a
r
a
m
e
t
e
r
f
o
l
l
o
w
s
:
                                10
x10
x10
a
r
r
a
y
=
c
o
n
c
```

(continues on next page)

(continued from previous page)

```
mixingtable

numberofscatteringangles= 2

crosssectionmessage
```

(continues on next page)

```
thresh
```

(continued from previous page)

```
mixture=     1
density(g/cc)=  19
.050

nuclide atom-dens.wgt.frac.zaawt
```

(continues on next page)

```
nuc
```



```
ide
```

(continued from previous page)

```
1092235  4
.39277
E
-02  9
.00000
E
-01  92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
m
o
d3 02
/28
/89
1092238  4
.81921
E
-03  1
.00000
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
U
N77
E
.
P
E
N
N
I
N
G
T
O
N
```

(continues on next page)

(continued from previous page)

```
m
i
x
t
u
r
e
=      2
d
e
n
s
i
t
y
(
g
/
c
c
)
= 0
.23509

n
u
c
l
i
d
e
a
t
o
m
-
d
e
n
s
.
w
g
t
.
f
r
a
c
.
z
a
a
w
t
n
u
c
l
i
d
e
```

(continues on next page)

(continued from previous page)

```
2001001  1
.57254
E
-02  1
.11927
E
-01   1001    1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1 11
/23
/92
2008016  7
.86270
E
-03  8
.88074
E
-01   8016   15
.9904   8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
```

(continues on next page)

```
o
n
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
*
*
*
```

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8.14.2 Array of Spheres in H_2O — Search on H_2O Density

This is the same problem as described above with the exception of the initial water density, which is now 0.25 gm/cc. A critical concentration search is performed on the water yielding a system k_{eff} = 1.0 for various densities of water. In the MORE search data, MIX=2 and SCNAME=H2O specify that the water component of mixture 2 is to be altered during the search from an initial value of 0.25 gm/cc. The maximum allowed density is ½ density water (0.5 gm/cc). The minimum allowed water density is 0.1 gm/cc.

The maximum constraint is calculated according to:

+CON= (5.0/0.25 1)/1.0 = 1.0

The minimum constraint is calculated according to:

CON= (0.1/0.25 1)/1.0 = 0.6

The search data and final search results for this problem follow:

```
=CSAS5S
10
x10
x10
A
R
R
A
Y
-
C
O
N
C
E
N
T
R
A
T
I
O
N
S
E
A
R
C
H

V7
-238

R
E
A
D
C
O
M
```

(continues on next page)

(continued from previous page)

```
U
R
A
N
I
U
M 1 1
.0  300
.0 92235 90
.0 92238 10
.0
E
N
D

H2
O     2 0
.25  300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
P
H
S
Q
U
A
R
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

S
P
H
E
R
E  1 1 2
.0

C
U
B
O
I
D  2 1 6
P4
.0

E
N
D
G
E
O
M
E
T
R
Y
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=10
N
U
Y
=10
N
U
Z
=10
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A
```

(continues on next page)

```
R
E
A
D
S
E
A
```

(continued from previous page)

```
A
L
T
E
R
M
I
X
=2
S
C
N
A
M
E
=
H2
O
f
a
c
t
o
r
=1
.0

-
C
O
N
=
-0
.6
+
C
O
N
=1
.0

E
N
D
S
E
A
R
C
H

E
N
D
```

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*
*
*
*
s
e
a
r
c
h
p
a
s
s  1
k
e
f
f
=  1
.02599
E
+00
+
o
r
-  1
.98346
E
-03
*
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```

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```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

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*
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*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
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i
t 95
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a
s
s  2
k
e
f
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=  6
.69203
E
-01
+
o
r
-  1
.55844
E
-03
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a
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a
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e
t
e
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w
a
s -6.00000E-01

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*m
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k
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v
d
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t
a
h
a
s
b
e
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r
e
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r
i
t
t
e
n
o
n
u
n
i
t 95
*
*
*
```

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*
*
*
s
e
a
r
c
h
p
a
s
s  3
k
e
f
f
=  1
.00197
E
+00
+
o
r
-  1
.73659
E
-03
*
*
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*
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```

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(continued from previous page)

```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s -4.37073E-02
                                10
x10
x10
a
r
r
a
y
-
c
o
n
c
e
n
t
r
a
t
i
o
n
s
e
a
r
c
h

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```

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```
*
*
*
```

(continued from previous page)

```
c
o
n
v
e
r
g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  3
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  -4.37073E-02

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
h
```

(continues on next page)

(continued from previous page)

```
k
-
e
f
f
=
+0
.00000
E
+00
+0
.00000
E
+00
*
p
+0
.00000
E
+00
*
p
*
*2
+0
.00000
E
+00
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  1
.00197
E
+00
+
o
r
-  1
.73659
E
-03
t
h
e
c
o
r
```

(continues on next page)

(continued from previous page)

```
                                    10
x10
x10
a
r
r
a
y
-
c
o
n
c
e
n
t
r
a
t
i
o
n
s
e
a
r
c
h

m
i
x
i
n
g
t
a
b
l
e


n
u
m
b
e
r
o
f
s
c
a
t
t
e
r
i
n
g
a
n
g
l
```

(continues on next page)

(continued from previous page)

```
c
r
o
s
s
s
e
c
t
i
o
n
m
e
s
s
a
g
e
t
h
r
e
s
h
o
l
d =5.7E-02

m
i
x
t
u
r
e
=     1
d
e
n
s
i
t
y
(
g
/
c
c
)
=  19
.050

n
u
c
l
i
d
e
a
t
```

(continues on next page)

(continued from previous page)

```
1092235  4
.39277
E
-02  9
.00000
E
-01  92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
m
o
d3 02
/28
/89
1092238  4
.81921
E
-03  1
.00000
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
U
N77
E
.
P
E
N
N
I
N
G
T
O
N
```

(continues on next page)

(continued from previous page)

```
m
i
x
t
u
r
e
=      2
d
e
n
s
i
t
y
(
g
/
c
c
)
= 0
.23864

n
u
c
l
i
d
e
a
t
o
m
-
d
e
n
s
.
w
g
t
.
f
r
a
c
.
z
a
a
w
t
n
u
c
l
i
d
e
```

(continues on next page)

(continued from previous page)

```
2001001  1
.59627
E
-02  1
.11926
E
-01   1001   1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1 11
/23
/92
2008016  7
.98136
E
-03  8
.88074
E
-01   8016  15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
```

(continues on next page)

```
o
n
```

(continued from previous page)

```
b
a
s
e
d
o
n
t
h
e
p
r
e
c
e
d
i
n
g
d
a
t
a
,
t
h
e
b
e
s
t
e
s
t
i
m
a
t
e
o
f
t
h
e
p
a
r
a
m
e
t
e
r
i
s    -4.37073E-02
```

(continues on next page)

(continued from previous page)

```
t
h
e
m
i
x
i
n
g
t
a
b
l
e
c
o
r
r
e
s
p
o
n
d
i
n
g
t
o
t
h
i
s
p
a
r
a
m
e
t
e
r
f
o
l
l
o
w
s
:
                                    10
x10
x10
a
r
r
a
y
c
o
n
```

(continues on next page)

(continued from previous page)

```
mixingtable

numberofscatteringangles= 2

crosssectionmessage
```

(continues on next page)

```
thresh
```

(continued from previous page)

```
m
i
x
t
u
r
e
=     1
d
e
n
s
i
t
y
(
g
/
c
c
)
=  19
.050

n
u
c
l
i
d
e
a
t
o
m
-
d
e
n
s
.
w
g
t
.
f
r
a
c
.
z
a
a
w
t
n
u
c
l
i
d
e
```

(continues on next page)

(continued from previous page)

```
1092235  4
.39277
E
-02  9
.00000
E
-01  92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
m
o
d3 02
/28
/89
1092238  4
.81921
E
-03  1
.00000
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
U
N77
E
.
P
E
N
N
I
N
G
T
O
N
```

(continues on next page)

(continued from previous page)

```
m
i
x
t
u
r
e
=      2
d
e
n
s
i
t
y
(
g
/
c
c
)
= 0
.23864

n
u
c
l
i
d
e
a
t
o
m
-
d
e
n
s
.
w
g
t
.
f
r
a
c
.
z
a
a
w
t
n
u
c
l
i
d
e
```

(continues on next page)

(continued from previous page)

```
2001001  1
.59627
E
-02  1
.11926
E
-01   1001    1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1 11
/23
/92
2008016  7
.98136
E
-03  8
.88074
E
-01   8016   15
.9904   8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
```

(continues on next page)

```
o
n
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
*
*
*
```

(continued from previous page)

8.14.3 UO_2F_2 Solution Tank — Critical Search on UO_2F_2 Density

Consider a large spherical tank partially filled with UO_2F_2 solution. The tank has a radius of 34.6 cm and is filled with solution to a height of 30.0 cm above the midpoint. The tank is composed of a 0.759 cm thick Al shell. The UO_2F_2 solution is composed of three standard compositions: UO2F2, HF acid, and H2O. The code combines these using a set algorithm. This may or may not produce a solution at the desired density. If the density of the solution is known it should be entered. Also, extra acid can be added to the solution by specifying a non-zero acid molarity.

A critical concentration search is performed on the water yielding system k_{eff} = 1.0 for various densities of UO_2F_2 in the solution. In the MORE search data, MIX=1 and SCNAME=UO2F2 specify that the UO_2F_2 component of the mixture 1 solution is to be altered during the search. The code calculates the density of the solution. The initial uranium fuel density is 300 gm/liter. The maximum allowed uranium density is 600 gm/liter. The minimum allowed uranium density is 150 gm/liter.

The maximum constraint is calculated according to:

+CON= (600/300 1)/1.0 = 1.0

The minimum constraint is calculated according to:

CON= (150/300 1)/1.0 = 0.5

The search data and final search results for this problem follow:

```
=CSAS5S

S
O
L
U
T
I
O
N
T
A
N
K
-
C
R
I
T
I
C
A
L
C
O
N
C
E
N
T
R
A
T
I
O
N
S
E
A
```

(continues on next page)

(continued from previous page)

```
V7
-238

R
E
A
D
C
O
M
P

S
O
L
N
U
O2
F2  1 300 0 1 300
.0 92235 4
.89 92238 95
.09 92234 0
.02
E
N
D

A
L          2 1
.0 300
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
G
E
O
M

H
E
M
I
S
P
H
E
-
Z  1 1 34
.6
```

(continues on next page)

(continued from previous page)

```
S
P
H
E
R
E      0 1 34
.6

S
P
H
E
R
E      2 1 34
.759

E
N
D
G
E
O
M

E
N
D
D
A
T
A

R
E
A
D
S
E
A
R
C
H
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C
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C
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T
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A
T
I
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A
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X
=1
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=
U
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F2
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A
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R
=1
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-
C
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-0
.5
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C
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s  1
k
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f
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=  8
.31461
E
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-  1
.14626
E
-03
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t
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a
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e
t
e
r
w
a
s  0.00000E+00

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d
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a
s
b
e
e
n
r
e
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r
i
t
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e
n
o
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u
n
i
t 99
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*
*
s
e
a
r
c
h
p
a
s
s  2
k
e
f
f
=  1
.05426
E
+00
+
o
r
-  1
.63141
E
-03
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t
h
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a
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a
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t
e
r
w
a
s  1.00000E+00

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d
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a
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e
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t 99
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*
*
*
s
e
a
r
c
h
p
a
s
s  3
k
e
f
f
=  1
.01773
E
+00
+
o
r
-  1
.42881
E
-03
*
*
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```

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```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  7.56451E-01

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*
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*
*
*m
o
d
i
f
i
e
d
k
e
n
o
v
d
a
t
a
h
a
s
b
e
e
n
r
e
w
r
i
t
t
e
n
o
n
u
n
i
t 95
*
*
*
```

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*
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*
s
e
a
r
c
h
p
a
s
s  4
k
e
f
f
=  9
.97887
E
-01
+
o
r
-  1
.42235
E
-03
*
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```
t
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a
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a
m
e
t
e
r
w
a
s  6.59454E-01

s
o
l
u
t
i
o
n
t
a
n
k
-
c
r
i
t
i
c
a
l
c
o
n
c
e
n
t
r
a
t
i
o
n
s
e
a
r
c
h
```

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```
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*
*
```

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```
*
*
*
```

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```
convergence was achieved on pass 4 the parameter was 6.59454E-01

the equation used in the
```

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```
k
-
e
f
f
=
+8
.31461
E
-01
+2
.45656
E
-01
*
p
+7
.41484
E
-02
*
p
*
*2
-9
.70021
E
-02
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  9
.97887
E
-01
+
o
r
-  1
.42235
E
-03
t
h
e
c
o
r
```

(continues on next page)

(continued from previous page)

```
s
o
l
u
t
i
o
n
t
a
n
k
-
c
r
i
t
i
c
a
l
c
o
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c
e
n
t
r
a
t
i
o
n
s
e
a
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c
h

m
i
x
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t
a
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n
u
m
b
e
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o
f
s
```

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```
c
r
o
s
s
s
e
c
t
i
o
n
m
e
s
s
a
g
e
t
h
r
e
s
h
o
l
d =5.7E-02



m
i
x
t
u
r
e
=     1
d
e
n
s
i
t
y
(
g
/
c
c
)
=  1
.5960

n
u
c
l
i
d
e
a
```

(continues on next page)

(continued from previous page)

```
 1001001  6
.36618
E
-02  6
.67438
E
-02   1001    1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1   11
/23
/92
 1008016  3
.43513
E
-02  5
.71507
E
-01   8016   15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
o
n
```

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(continued from previous page)

```
 1009019  2
.52040
E
-03  4
.98199
E
-02   9019   18
.9982  9
f 19
o
r
n
l
e
v
a
l
j
u
l74
c
.
y
.
f
u
d
.
c
.
l
a
r
s
m
o
d3
 12
/16
/88
 1092234  2
.56198
E
-07  6
.23860
E
-05  92234  234
.0405  92
U234
B
N
L
H
E
D
L
+
```

(continues on next page)

```
E
V
A
L
J
U
L78
```

(continued from previous page)

```
 01
/10
/91
 1092235  6
.23730
E
-05  1
.52534
E
-02  92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
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r
.
b
h
a
t
m
o
d3 02
/28
/89
 1092238  1
.19757
E
-03  2
.96614
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
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U
N77
E
.
P
E
N
N
I
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G
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(continued from previous page)

```
 02
/13
/92


m
i
x
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=     2
d
e
n
s
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y
(
g
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c
c
)
=  2
.7020

n
u
c
l
i
d
e
a
t
o
m
-
d
e
n
s
.
w
g
t
.
f
r
a
c
.
z
a
a
w
t
```

(continues on next page)

```
n
u
c
l
.
```

(continued from previous page)

```
 2013027  6
.03066
E
-02  1
.00000
E
+00  13027  26
.9818  13
a
l 270
l
a
s
l
e
v
a
l
d
e
c73
p
.
g
.
y
o
u
n
g
d
.
g
m
o
d1
 11
/29
/88


b
a
s
e
d
o
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c
e
d
i
n
g
d
a
t
a
```

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a
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s
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o
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o
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t
a
n
```

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(continued from previous page)

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n
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m
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e
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f
s
c
a
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t
e
r
i
n
g
a
n
g
l
e
s
=   2

c
r
o
s
s
s
e
c
t
i
o
n
m
e
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s
a
g
e
t
h
r
e
s
```

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```
m
i
x
t
u
r
e
=     1
d
e
n
s
i
t
y
(
g
/
c
c
)
=  1
.5998

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u
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i
d
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n
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.
w
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.
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.
z
a
a
w
t
n
u
c
l
i
d
e
```

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(continued from previous page)

```
 1001001  6
.36618
E
-02  6
.65852
E
-02   1001    1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1  11
/23
/92
 1008016  3
.43662
E
-02  5
.70395
E
-01   8016   15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
o
n
```

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(continued from previous page)

```
 1009019  2
.53528
E
-03  4
.99948
E
-02   9019   18
.9982  9
f 19
o
r
n
l
e
v
a
l
j
u
l74
c
.
y
.
f
u
d
.
c
.
l
a
r
s
m
o
d3
 12
/16
/88
 1092234  2
.57710
E
-07  6
.26050
E
-05  92234  234
.0405  92
U 234
B
N
L
H
E
D
L
+
E
V
A
L
J
U
L78
```

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```
 01
/10
/91
 1092235  6
.27412
E
-05  1
.53069
E
-02  92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
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d3 02
/28
/89
 1092238  1
.20464
E
-03  2
.97655
E
-01  92238  238
.0510  92
U 238
A
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+
E
V
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J
U
N77
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```
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/92


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y
(
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/
c
c
)
=  2
.7020

n
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m
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z
a
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```
 2013027  6
.03066
E
-02  1
.00000
E
+00  13027   26
.9818  13
a
l 270
l
a
s
l
e
v
a
l
d
e
c73
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g
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y
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g
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d1
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/29
/88


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The final solution for this search contains 500 gm/liter of uranium. The search, however, did not change the amount of acid or water in the solution. To get a better estimation of the solution density and k_{eff} for this concentration of uranium the problem should be run again with an initial uranium density of 500 gm/liter as shown below.

8.14.4 UO_2F_2 Solution Tank — Critical Search on UO_2F_2 Density, Check

This is the same UO_2F_2 solution tank problem examined above except the initial uranium density is 500 gm/liter. This problem is run again so the code will calculate water and acid densities associated with this density of uranium. The search data has also been modified to account for the new density of uranium.

A critical concentration search is performed on the water yielding system k_{eff} = 1.0 for various densities of UO_2F_2 in the solution. In the MORE search data, MIX=1 and SCNAME=UO2F2 specify that the UO_2F_2 component of the mixture 1 solution is to be altered during the search. The code calculates the density of the solution. The initial uranium fuel density is 500 gm/liter. The maximum allowed uranium density is 600 gm/liter. The minimum allowed uranium density is 400 gm/liter.

The maximum constraint is calculated according to:

+CON= (600/500 1)/1.0 = 0.2

The minimum constraint is calculated according to:

CON= (400/500 1)/1.0 = 0.2

The search data and final search results for this problem follow:

```
=csas5s

s
o
l
u
t
i
o
n
t
a
n
k
-
c
r
i
t
i
c
a
l
c
o
n
c
e
n
t
```

(continues on next page)

```
r
a
t
i
o
n
s
```

(continued from previous page)

```
v7
-238
read
 comp

s
o
l
n
u
o2
f2  1 500 0 1 300
.0 92235 4
.89 92238 95
.09 92234 0
.02 end

a
l         2 1
.0 300
.0 end
end
 comp
read
 geom

h
e
m
i
s
p
h
e
-
z  1 1 34
.6
c
h
o
r
d 30
.

s
p
h
e
r
e      0 1 34
.6

s
p
h
e
r
e      2 1 34
.759
```

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```
end
 geom
end
 data

R
E
A
D
S
E
A
R
C
H
C
R
I
T
I
C
A
L
C
O
N
C
E
N
T
R
A
T
I
O
N
K
E
F
=1
.0
M
O
R
E

A
L
T
E
R
M
I
X
=1
S
C
N
A
M
E
=
u
o2
```

(continues on next page)

(continued from previous page)

```
-
C
O
N
=
-0
.2
+
C
O
N
=0
.2

E
N
D
S
E
A
R
C
H
end
```

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*
*
s
e
a
r
c
h
p
a
s
s  1
k
e
f
f
= 9
.99662
E
-01
```

(continues on next page)

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```
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s  0.00000E+00

s
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l
u
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o
n
t
a
n
k
-
c
r
i
t
i
c
a
l
c
o
n
c
e
n
t
r
a
t
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o
n
s
e
a
r
c
h
```

(continues on next page)

(continued from previous page)

```
*
*
*
```

(continued from previous page)

```
c
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v
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g
e
n
c
e
w
a
s
a
c
h
i
e
v
e
d
o
n
p
a
s
s  1
t
h
e
p
a
r
a
m
e
t
e
r
w
a
s   0.00000E+00

t
h
e
e
q
u
a
t
i
o
n
u
s
e
d
i
n
t
```

(continues on next page)

(continued from previous page)

```
k
-
e
f
f
=
+0
.00000
E
+00
+0
.00000
E
+00
*
p
+0
.00000
E
+00
*
p
*
*2
+0
.00000
E
+00
*
p
*
*3


k
-
e
f
f
e
c
t
i
v
e
=  9
.99662
E
-01
+
o
r
-  1
.40567
E
-03
t
h
e
c
o
r
```

(continues on next page)

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```
s
o
l
u
t
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o
n
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a
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k
-
c
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i
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c
a
l
c
o
n
c
e
n
t
r
a
t
i
o
n
s
e
a
r
c
h

m
i
x
i
n
g
t
a
b
l
e


n
u
m
b
e
r
o
f
s
```

(continues on next page)

(continued from previous page)

```
c
r
o
s
s
s
e
c
t
i
o
n
m
e
s
s
a
g
e
t
h
r
e
s
h
o
l
d =5.7E-02

m
i
x
t
u
r
e
=     1
d
e
n
s
i
t
y
(
g
/
c
c
)
=  1
.5656

n
u
c
l
i
d
e
a
t
```

(continues on next page)

(continued from previous page)

```
 1001001  6
.14448
E
-02  6
.56680
E
-02   1001    1
.0077
h
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r 1301
/1002
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/23
/92
 1008016  3
.32538
E
-02  5
.63969
E
-01   8016   15
.9904  8
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```
 1009019  2
.53136
E
-03  5
.10061
E
-02   9019   18
.9982  9
f 19
o
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n
l
e
v
a
l
j
u
l74
c
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y
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m
o
d312
/16
/88
 1092234  2
.57312
E
-07  6
.38714
E
-05  92234  234
.0405  92
U 234
B
N
L
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D
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J
U
L78
```

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```
 01
/10
/91
 1092235  6
.26441
E
-05  1
.56166
E
-02  92235  235
.0441  92
u 235
b
n
l
e
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l
a
p
r77
m
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b
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o
d3 02
/28
/89
 1092238  1
.20278
E
-03  3
.03676
E
-01  92238  238
.0510  92
U 238
A
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.7020

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 2013027  6
.03066
E
-02  1
.00000
E
+00  13027   26
.9818  13
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c73
p
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g
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y
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/29
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```
mixingtable

numberofscatteringangles= 2

crosssectionmessage
```

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 1001001  6
.14448
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-02  6
.56680
E
-02   1001    1
.0077
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/1002
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d1 11
/23
/92
 1008016  3
.32538
E
-02  5
.63969
E
-01   8016   15
.9904  8
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```
 1009019  2
.53136
E
-03  5
.10061
E
-02   9019   18
.9982  9
f 19
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 12
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/88
 1092234  2
.57312
E
-07  6
.38714
E
-05  92234  234
.0405  92
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 1092235  6
.26441
E
-05  1
.56166
E
-02  92235  235
.0441  92
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/89
 1092238  1
.20278
E
-03  3
.03676
E
-01  92238  238
.0510  92
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=  2
.7020

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 2013027  6
.03066
E
-02  1
.00000
E
+00  13027   26
.9818  13
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This problem converged on the first pass, so the amount of uranium, HF acid, and water in the solution were reasonably good estimates. For this problem the HF acid and H_2O only changed marginally and, therefore, had very little effect on the system k_{eff}. This is not always the case; therefore if a search is being done on a solution, the problem should always be rerun with the final search densities.

8.14.5 Fuel Bundles Separated by Flux Traps — Critical Search Boron and Al Densities

The fuel bundles in this problem represent 17 × 17 PWR fuel assemblies. The fuel pins are smeared together, making a mixture 100. The fuel pins consist of 4.35 wt % ^{235}U having a diameter of 0.823 cm, zirconium cladding having an outer diameter of 0.9627 cm, and a pitch of 1.275 cm. The fuel bundle is represented as a 10.8375 cm × 10.8375 cm × 366 cm cuboid of mixture 100 surrounded by Boral and then water. The Boral has a density of 2.61 g/cm^3 and has an initial composed of 50.0 wt % B_4C and 50.0 wt % Al. The fuel bundles are at a fixed pitch of 13.0 cm. Boral plates surrounding the X and Y sides of each fuel assembly are 0.1625 cm thick. Full density water is between the Boral plates.

A critical concentration search is performed on the Boral plates searching for a system k_{eff} = 0.95. The Boral plates are at a fixed density of 2.61 gm/cc. As the density of the B_4C changes, the density of the Al changes in the opposite direction maintaining a constant Boral density. There are two entries in the MORE search data. The first entry, MIX=4 SCNAME=b4c factor=1.0 specifies that the B_4C of mixture 4 is to be altered during the search. The second entry, MIX=4 SCNAME=al factor = 1.0 specifies that aluminum is to be changed in the opposite direction and proportionally to B_4C during the search. Both B_4C and Al have the same initial density of 0.5 * 2.61 = 1.305 gm/cc.

The maximum constraint is calculated according to:

+CON= (2.59695/1.305 1)/1.0 = 0.99

The minimum constraint is calculated according to:

CON= (0.1305/1.305 1)/1.0 = 0.9

The search data and final search results for this problem follow:

```
=csas5s

a
r
r
a
y
o
f
f
u
e
l
b
u
n
d
l
e
s
w
i
```

(continues on next page)

```
t
h
f
l
u
x
t
```

(continued from previous page)

```
v7
-238
read
 comp

u
o2    1
.84 300
.  92235 4
.35 92238 95
.65 end

z
r     2 1 end

h2
o    3 1 end

b4
c    4
d
e
n
=2
.61  0
.5  end

a
l     4
d
e
n
=2
.61 0
.5 end

h2
o    5 1
.0 end
end
 comp
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
```

(continues on next page)

```
q
u
a
r
e
p
i
```

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```
end
 celldata
read
 param
 far
=yes
 gen
=
2
0
3
 npg
=
1
0
0
0
 end
 param
read
 geom

g
l
o
b
a
l
u
n
i
t 1

c
u
b
o
i
d 100 1 4
p10
.8375 2
p183
.0

c
u
b
o
i
d   4 1 4
p11
.0    2
p183
.0

c
u
b
o
i
d   5 1 4
p13
.0    2
p183
```

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```
end
 geom
read
 bounds
 xfc
=mirror
 yfc
=mirror
 end
 bounds
end
 data
read
 search

 critical
 concentration

 kef
=
0
.
9
5
 more

a
l
t
e
r
m
i
x
=4
s
c
n
a
m
e
=
a
r
b
m
b4
c
f
a
c
t
o
r
=1
.0
```

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```
a
l
t
e
r
m
i
```

(continued from previous page)

```
-
c
o
n
=
-0
.9
+
c
o
n
=0
.99
end
 search
end
```

```
=csas5s

a
r
r
a
y
o
f
f
u
e
l
b
u
n
d
l
e
s
w
i
t
h
f
l
u
x
t
r
a
p

v7
-238
read
 comp

u
o2    1
.84 300
    92235 4
.35 92238 95
.65 end
```

(continues on next page)

(continued from previous page)

```
z
r      2 1 end

h2
o     3 1 end

b4
c     4
d
e
n
=2
.61   0
.5   end

a
l      4
d
e
n
=2
.61 0
.5 end

h2
o     5 1
.0 end
end
 comp
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
q
u
a
r
e
p
i
t
c
h
p
i
t
c
h
=1
.275 3
f
u
```

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```
end
 celldata
read
 param
 far
=yes
 gen
=
2
0
3
 npg
=
1
0
0
0
 end
 param
read
 geom

g
l
o
b
a
l
u
n
i
t 1

c
u
b
o
i
d 100 1 4
p10
.8375 2
p183
.0

c
u
b
o
i
d   4 1 4
p11
.0    2
p183
.0

c
u
b
o
i
d   5 1 4
p13
.0    2
p183
```

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```
end
 geom
read
 bounds
 xfc
=mirror
 yfc
=mirror
 end
 bounds
end
 data
read
 search

 critical
 concentration

 kef
=
0
.
9
5
 more

a
l
t
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=4
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e
=
a
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b
m
b4
c
f
a
c
t
o
r
=1
.0
```

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```
a
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m
i
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-0
.9
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=0
.99
end
 search
end


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f
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.22991
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-01
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r
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.79474
E
-03
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s  0.00000E+00

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p
m
m
e
s
h
i
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m
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s
h
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i
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z
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    4
m
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e  2
   14
m
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i
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a
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s
i
n
z
o
n
e  3

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*m
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d
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f
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e
d
k
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v
d
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t
a
h
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*
*
s
e
a
r
c
h
p
a
s
s  6
k
e
f
f
=  9
.48930
E
-01
+
o
r
-  1
.69920
E
-03
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t
h
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a
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a
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e
r
w
a
s -8.65663E-01

a
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c
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p
a
s
s  6
t
h
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p
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m
e
t
e
r
w
a
s  -8.65663E-01

t
h
e
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q
u
a
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s
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d
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n
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h
```

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```
k
-
e
f
f
=
+8
.66738
E
-01
+2
.74121
E
-01
*
p
+5
.80563
E
-02
*
p
*
*2
-4
.25484
E
-01
*
p
*
*3


k
-
e
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i
v
e
=  9
.48930
E
-01
+
o
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-  1
.69920
E
-03
t
h
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c
o
r
```

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a
r
r
a
y
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n
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a
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c
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c
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m
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t
h
r
e
s
h
o
l
d =5.7E-02

m
i
x
t
u
r
e
=     1
d
e
n
s
i
t
y
(
g
/
c
c
)
=  9
.2064

n
u
c
l
i
d
e
a
t
```

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(continued from previous page)

```
 1008016  4
.10835
E
-02  1
.18491
E
-01   8016  15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
o
n
 1092235  9
.04496
E
-04  3
.83457
E
-02  92235 235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
```

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```
m
o
d3 02
/28
/89
```

(continued from previous page)

```
 1092238  1
.96373
E
-02  8
.43163
E
-01  92238 238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
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N77
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.
P
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I
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T
O
N
M
O
D3 02
/13
/92


m
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e
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g
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=
.4900
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l
e
 2040000  4
.28457
E
-02  1
.00000
E
+00  40000  91
.2196  40
z
r
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e
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a
l
a
p
r76
```

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m
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y
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c
c
)
= 0
.99817

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z
a
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c
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i
d
e
```

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```
 3001001  6
.67692
E
-02  1
.11927
E
-01   1001   1
.0077
h
y
d
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o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1   11
/23
/92
 3008016  3
.33846
E
-02  8
.88074
E
-01   8016  15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
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a
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o
n
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m
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y
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=  2
.6100

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z
a
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c
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```
 4005010  1
.52119
E
-03  9
.69077
E
-03  5010  10
.0130   5
b100
l
a
s
l
e
v
a
l
d
e
c76
g
.
h
a
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e
l
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s
t
e
w
a
r
t
m
o
d1  12
/11
/92
 4005011  6
.12300
E
-03  4
.28888
E
-02  5011  11
.0096 5
b11
g
e
b
n
l
e
v
a
l
s
e
p71
c
.
c
```

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```
 4006012  1
.91105
E
-03  1
.45903
E
-02  6000  12
.0001 6
c
o
r
n
l
e
v
a
l
d
e
c73
c
.
y
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f
u
a
n
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g
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p
e
r
e
y
m
o
d2 12
/11
/92
 4013027  5
.43405
E
-02  9
.32830
E
-01 13027  26
.9818 13
a
l270
l
a
s
l
```

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e
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c73
```

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m
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```
 5001001  6
.67692
E
-02  1
.11927
E
-01   1001    1
.0077
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r 1301
/1002
m
o
d1 11
/23
/92
 5008016  3
.33846
E
-02  8
.88074
E
-01   8016   15
.9904  8
O 16
f
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m
v
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.0000

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c
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i
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```

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```
 3001001  0
.00000
E
+00  0
.00000
E
+00   1001    1
.0077
h
y
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a
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r 1301
/1002
m
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d1 11
/23
/92
 3008016  0
.00000
E
+00  0
.00000
E
+00   8016   15
.9904  8
O 16
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```
 1008016  0
.00000
E
+00  0
.00000
E
+00   8016   15
.9904  8
O 16
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n
 2040000  0
.00000
E
+00  0
.00000
E
+00  40000   91
.2196  40
z
r
s
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e
v
a
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a
p
r76
m
.
d
r
a
k
e
d
.
s
a
m
o
d2 01
```

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```
 1092235  0
.00000
E
+00  0
.00000
E
+00  92235  235
.0441  92
u 235
b
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e
v
a
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p
r77
m
.
r
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b
h
a
t
m
o
d3 02
/28
/89
 1092238  0
.00000
E
+00  0
.00000
E
+00  92238  238
.0510  92
U 238
A
N
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E
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J
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N77
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P
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 02
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/92



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```
mixingtable

numberofscatteringangles= 2

crosssectionmessage
```

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```
thresh
```

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m
i
x
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=     1
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.2064

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```
 1008016  4
.10835
E
-02  1
.18491
E
-01   8016   15
.9904  8
O 16
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v
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r
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n 6
e
v
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n
 1092235  9
.04496
E
-04  3
.83457
E
-02  92235  235
.0441  92
u 235
b
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b
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```

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```
m
o
d3 02
/28
/89
```

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```
 1092238  1
.96373
E
-02  8
.43163
E
-01  92238  238
.0510  92
U 238
A
N
L
+
E
V
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D3 02
/13
/92


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c
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.4900
```

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l
e
 2040000  4
.28457
E
-02  1
.00000
E
+00  40000   91
.2196  40
z
r
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a
l
a
p
r76
```

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m
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y
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c
)
= 0
.99817

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```

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```
 3001001  6
.67692
E
-02  1
.11927
E
-01   1001    1
.0077
h
y
d
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o
g
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i
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w
a
t
e
r 1301
/1002
m
o
d1   11
/23
/92
 3008016  3
.33846
E
-02  8
.88074
E
-01   8016   15
.9904  8
O 16
f
r
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m
v
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m
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x
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e
=      4
d
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y
(
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c
c
)
=  2
.6100

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```

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```
 4005010  1
.50619
E
-03  9
.59518
E
-03   5010   10
.0130 5
b 100
l
a
s
l
e
v
a
l
d
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c76
g
.
h
a
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e
l
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s
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e
w
a
r
t
m
o
d1 12
/11
/92
 4005011  6
.06261
E
-03  4
.24657
E
-02   5011   11
.0096 5
b11
g
e
b
n
l
e
v
a
```

(continues on next page)

```
l
s
e
p71
c
.
c
```

(continued from previous page)

```
 4006012  1
.89220
E
-03  1
.44464
E
-02   6000   12
.0001 6
c
o
r
n
l
e
v
a
l
d
e
c73
c
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y
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f
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p
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e
y
m
o
d2 12
/11
/92
 4013027  5
.43791
E
-02  9
.33493
E
-01  13027   26
.9818  13
a
l 270
l
a
s
l
```

(continues on next page)

```
e
v
a
l
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e
c73
```

(continued from previous page)

```
m
i
x
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=      5
d
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= 0
.99817

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```

(continues on next page)

(continued from previous page)

```
 5001001  6
.67692
E
-02  1
.11927
E
-01   1001    1
.0077
h
y
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r 1301
/1002
m
o
d1   11
/23
/92
 5008016  3
.33846
E
-02  8
.88074
E
-01   8016   15
.9904  8
O 16
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m
i
x
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d
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n
s
i
t
y
(
g
/
c
c
)
=  0
.0000

n
u
c
l
i
d
e
a
t
o
m
-
d
e
n
s
.
w
g
t
.
f
r
a
c
.
z
a
a
w
t
n
u
c
l
i
d
e
```

(continues on next page)

(continued from previous page)

```
 3001001  0
.00000
E
+00  0
.00000
E
+00   1001    1
.0077
h
y
d
r
o
g
e
n
i
n
w
a
t
e
r 1301
/1002
m
o
d1   11
/23
/92
 3008016  0
.00000
E
+00  0
.00000
E
+00   8016   15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
```

(continues on next page)

```
o
n
```

(continued from previous page)

```
 1008016  0
.00000
E
+00  0
.00000
E
+00    8016  15
.9904  8
O 16
f
r
o
m
v
e
r
s
i
o
n 6
e
v
a
l
u
a
t
i
o
n
 2040000  0
.00000
E
+00  0
.00000
E
+00   40000  91
.2196  40
z
r
s
a
i
e
v
a
l
a
p
r76
m
.
d
r
a
k
e
d
.
s
a
m
o
d2 01
```

(continues on next page)

(continued from previous page)

```
 1092235  0
.00000
E
+00  0
.00000
E
+00   92235  235
.0441  92
u 235
b
n
l
e
v
a
l
a
p
r77
m
.
r
.
b
h
a
t
m
o
d3 02
/28
/89
 1092238  0
.00000
E
+00  0
.00000
E
+00   92238  238
.0510  92
U 238
A
N
L
+
E
V
A
L
J
U
N77
E
.
P
E
N
N
I
N
G
T
O
N
```

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```
*
*
*
```

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```
*
*
*
```

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CHAPTER

NINE

CSAS6: CONTROL MODULE FOR ENHANCED CRITICALITY SAFETY ANALYSIS WITH KENO-VI

L. M. Petrie, K. B. Bekar, D. F. Hollenbach,[1] *S. Goluoglu*[1]

The **C**riticality **S**afety **A**nalysis **S**equence with KENO-VI (CSAS6) provides reliable and efficient means of performing *keff* calculations for systems that are routinely encountered in engineering practice. In the multigroup calculation mode, CSAS6 uses XSProc to process the cross sections for temperature corrections and problem-dependent resonance self-shielding and calculates the *keff* of three-dimensional (3-D) system models. If the continuous energy calculation mode is selected no resonance processing is needed and the continuous energy cross sections are used directly in KENO-VI, with temperature corrections provided as the cross sections are loaded. The geometric modeling capabilities available in KENO-VI coupled with the automated cross-section processing within the control sequences allow complex, 3-D systems to be easily analyzed.

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ACKNOWLEDGMENTS

The CSAS6 Criticality Safety Analysis Sequence is based on the CSAS control module, and the KENO-VI functional module, described in their respective chapters. G. E. Whitesides is acknowledged for his contributions through early versions of KENO. Appreciation is expressed to C. V. Parks and S. M. Bowman for their guidance in developing CSAS6.

9.1 Introduction

Criticality Safety Analysis Sequence with KENO-VI (CSAS6) provides reliable and efficient means of performing *keff* calculations for systems that are routinely encountered in engineering practice, especially in the calculation of *keff* of three-dimensional (3-D) system models. CSAS6 implements XSProc to process material input and provide a temperature and resonance-corrected cross-section library based on the physical characteristics of the problem being analyzed. If a continuous energy cross-section library is specified, no resonance processing is needed and the continuous energy cross sections are used directly in KENO-VI, with temperature corrections provided as the cross sections are loaded.

9.2 Sequence Capabilities

CSAS6 is designed to prepare a resonance-corrected cross-section library for subsequent use in KENO-VI. In order to minimize human error, the SCALE data handling is automated as much as possible. CSAS6 and many other SCALE sequences apply a standardized procedure to provide appropriate number densities and cross sections for the calculation. XSProc is responsible for reading the standard composition data and other engineering-type specifications, including volume fraction or percent theoretical density, temperature, and isotopic distribution as well as the unit cell data. XSProc then generates number densities and related information, prepares geometry data for resonance self-shielding and flux-weighting cell calculations, if needed, and (if needed) provides problem-dependent multigroup cross-section processing. CSAS6 invokes a KENO-VI Data Processor to read and check the KENO-VI data. When the data checking has been completed, the control sequence executes XSProc to prepare a resonance-corrected microscopic cross-section library in the AMPX working library format if a multigroup library has been selected.

For each unit cell specified as being cell-weighted, XSProc performs the necessary calculations and produces a cell-weighted microscopic cross-section library. KENO-VI may be executed to calculate the *keff* or neutron multiplication factor using the cross-section library that was prepared by the control sequence.

9.3 Multigroup CSAS6 limitations

The CSAS6 control module was developed to use simple input data and prepare problem-dependent cross sections for use in calculating the effective neutron multiplication factor of a 3-D system using KENO-VI and possibly XSDRNPM. An attempt was made to make the system as general as possible within the constraints of the standardized methods chosen to be used in SCALE. Standardized methods of data input were adopted to allow easy data entry and for quality assurance purposes. Some of the limitations of the CSAS6 sequence are a result of using preprocessed multigroup cross sections. Inherent limitations in CSAS6 are as follows:

1. Two-dimensional (2-D) effects such as fuel rods in assemblies where some positions are filled with control rod guide tubes, burnable poison rods and/or fuel rods of different enrichments. The cross sections are processed as if the rods are in an infinite lattice of rods. If the user inputs a Dancoff factor for the cell (such as one computed by MCDancoff), XSProc can produce an infinite lattice cell, which reproduces that Dancoff. This can mitigate some two dimensional lattice effects.

It is strongly recommended that the user perform CSAS6 calculations of benchmark experiments similar to the problem of interest to demonstrate the validity of the cross-section data and processing for that type of problem.

9.3.1 Continuous energy CSAS6 limitations

When continuous energy KENO calculations are desired, none of the resonance processing modules are applicable or needed. Moreover, the MG limitations noted in the previous section are eliminated. The continuous energy cross sections are directly used in KENO. An existing multigroup input file can easily be converted to a continuous energy input file by simply specifying the continuous energy library. In this case, all cell data is ignored. However, the following limitations exist:

1. If CELLMIX is defined in the cell data, the problem will not run in the continuous energy mode. CELLMIX implies new mixture cross sections are generated using XSDRNPM-calculated cell fluxes and therefore is not applicable in the continuous energy mode.
2. Only VACUUM, MIRROR, PERIODIC, and WHITE boundary conditions are allowed. Other albedos, e.g., WATER, CARBON, POLY, etc. are for multigroup only.
3. Problems with DOUBLEHET cell data are not allowed as they inherently utilize CELLMIX feature.

9.4 Input Data Guide

The input data for CSAS6 are composed of two broad categories of data. The first is XSProc, including Standard Composition Specification Data and Unit Cell Geometry Specification. This first category specifies the cross-section library and defines the composition of each mixture and optionally the unit cell geometry that may be used to process the cross sections. The second category of data, the KENO-VI input data, is used to specify the geometric and boundary conditions that represent the physical 3-D configuration of the problem. Both data blocks are necessary for CSAS6.

All data are entered in free form, allowing alphanumeric data, floating-point data, and integer data to be entered in an unstructured manner. Up to 252 columns of data entry per line are allowed. Data can usually start or end in any column with a few exceptions. As an example, the word END beginning in column 1 and followed by two blank spaces or a new line will end the problem and any data following will be ignored. Each data entry must be followed by one or more blanks to terminate the data entry. For numeric data, either a comma or a blank can be used to terminate each data entry. Integers may be entered for floating values. For example, 10 will be interpreted as 10.0. Imbedded blanks are not allowed within a data entry unless an E precedes a single blank as in an unsigned exponent in a floating-point number. For example, 1.0E 4 would be correctly interpreted as 1.0×10^4.

The word "END" is a special data item. An "END" may have a name or label associated with it. The name or label associated with an "END" is separated from the "END" by a single blank and is a maximum of 12 characters long. *At least two blanks or a new line MUST follow every labeled and unlabeled "END." It is the user's responsibility to ensure compliance with this restriction. Failure to observe this restriction can result in the use of incorrect or incomplete data without the benefit of warning or error messages.*

Multiple entries of the same data value can be achieved by specifying the number of times the data value is to be entered, followed by either R, *, or $, followed by the data value to be repeated. Imbedded blanks are not allowed between the number of repeats and the repeat flag. For example, 5R12, 5*12, 5$12, or 5R 12, etc., will enter five successive 12s in the input data. Multiple zeros can be specified as nZ where n is the number of zeroes to be entered.

The purpose of this section is to define the input data in discrete subsections relating to a particular type of data. Tables of the input data are included in each subsection, and the entries are described in more detail in the appropriate sections.

Resonance-corrected cross sections are generated using the appropriate boundary conditions for the unit cell description (i.e., void for the outer surface of a single unit, white for the outer surface of an infinite array of cylinders, spheres, or planes). As many unit cells as needed may be specified in a problem. A unit cell is cell-weighted by using the keyword CELLMIX= followed by a unique user specified mixture number in the unit cell data.

To check the input data without actually processing the cross sections, the words "PARM=CHECK" or "PARM=CHK" should be entered, as shown below.

```
=CSAS6 PARM=CHK
```

or

```
#CSAS6 PARM=CHK
```

This will cause the input data for CSAS6 to be checked and appropriate error messages to be printed. If plots are specified in the data, they will be printed. This feature allows the user to debug and verify the input data while using a minimum amount of computer time.

9.4.1 XSProc data

The XSProc reads the standard composition specification data and the unit cell geometry specifications. It then produces the mixing table and unit cell information necessary for processing the cross sections if needed. The XSProc section of this manual provides a detailed description of the input data and processing options.

9.4.2 KENO-VI data

Table 9.1 contains the outline for the KENO-VI input. The KENO-VI input is divided into 13 data blocks. A brief outline of commonly used data blocks is shown in Table 9.1. Note that parameter data must precede all other KENO data blocks. Information on all KENO-VI input is provided in the KENO chapter of this document and will not be repeated here.

Table 9.1: Outline of KENO data

Type of data	**Starting flag**	**Comments**	**Termination flag**
Parameters*	READ PARAMETER	Enter desired parameter data	END PARAMETER
Geometry	READ GEOMETRY	Enter desired geometry data	END GEOMETRY
Array data	READ ARRAY	Enter desired array data	END ARRAY
Boundary conditions	READ BOUNDS	Enter desired boundary conditions	END BOUNDS
Energy group boundaries	READ ENERGY	Enter desired neutron energy group boundaries	END ENERGY
Start data or initial source	READ START	Enter desired start data	END START
Plot data	READ PLOT	Enter desired plot data	END PLOT
Grid geometry data	READ GRID	Enter desired mesh data	END GRID
Reaction	READ REACTION	Enter desire reaction tallies (CE mode only)	END REACTION
KENO-VI data terminus	END DATA	Enter to signal the end of all KENO-VI data	
*Must precede all other data blocks in this table.			

9.5 Sample Problems

This section contains sample problems to demonstrate some of the options available in CSAS6. A brief problem description and the associated input data for multigroup mode of calculation are included for each problem. The same sample problems may be executed in the continuous energy mode by changing the library name to an continuous-energy library. See Appendix A (SECTIONREFERENCE) for additional examples.

9.5.1 Sample Problem 1: Aluminum 30 Degree Pipe Angle Intersection

The purpose of this problem is to calculate the k-effective of a system composed of intersecting aluminum pipes, in the shape of a Y, filled with a 5% enriched UO_2F_2 solution. The UO_2F_2 solution at 299°K contains 907.0 gm/l of uranium, no excess acid, and has a specific gravity of 2.0289 gm/cm^3. The assembly is composed of a 212.1 cm long vertical pipe and a second pipe that intersects the vertical pipe 76.7 cm from the outside bottom at an angle of 29.26 degrees with the upper vertical pipe. Both pipes have 13.95 cm inner diameters and 14.11 cm outer diameters. The vertical pipe is open on the top and 1.3 cm thick on the bottom. The Y-leg pipe, in the YZ-plane, is 126.04 cm in length with the sealed end 0.64 cm thick. The assembly is filled with solution to a height 129.5 cm above the outside bottom of the vertical pipe. From the point where the pipes intersect the assembly is surrounded by water 37.0 cm in the ±X directions, 100 cm in the +Y direction, –37 cm in the –Y direction, to the top of the assembly in the +Z direction, and –99.6 cm in the –Z direction.

```
=csas6

s
a
m
p
l
e
p
r
o
b
l
e
m 1
Y
-30
, 5
%
u
o2
f2
, 907
.0
g
/
l
, 128
.2
,
s
o
l
n
.
h
t
.

v7
-238
read
 comp

s
o
l
t
i
o
n
```

(continues on next page)

Fig. 9.1: Critical assembly of UO_2F_2 solution in a 30°-Y aluminum pipe.

(continued from previous page)

```
m
i
x
=1

r
h
o
[
u
o2
f2
]
=907
.0 92235 5
.0 92238 95
.0

d
e
n
s
i
t
y
=
?

t
e
m
p
e
r
a
t
u
r
e
=299
.0
  end
 solution

a
l        2 1
.0 end

h2
o       3 1
.0 end
end
 comp
read
 parameters
```

(continues on next page)

```
f
l
x
=
y
e
s
```

(continued from previous page)

```
end
 parameters
read
 start

n
s
t
=6
t
f
x
=0
.0
t
f
y
=0
.0
t
f
z
=0
.0
l
n
u
=1000
end
 start
read
 geometry

g
l
o
b
a
l

u
n
i
t 1

c
o
m
='30 deg y'

c
y
l
i
n
d
e
r 10  13
.95  135
.4
.75
.4
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r 20  14
.11  135
.4
-76
.7

c
y
l
i
n
d
e
r 30  13
.95  125
.4   0
.0
r
o
t
a
t
e
a2
=
-29
.26

c
y
l
i
n
d
e
r 40  14
.11  126
.04  0
.0
r
o
t
a
t
e
a2
=
-29
.26
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d   50  2
p37
.0 100
.
-37
.0 52
.8
-75
.4

c
u
b
o
i
d   60  2
p37
.0 100
.
-37
.0 135
.4
-99
.6

m
e
d
i
a  1  1 10  50

m
e
d
i
a  2  1 20
-10
-30

m
e
d
i
a  1  1 30  50
-10

m
e
d
i
a  2  1 40
-30
-20
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  0  1 10
-50

m
e
d
i
a  0  1 30
-50
-10

m
e
d
i
a  3  1 60
-20
-40
-10

b
o
u
n
d
a
r
y  60
end
 geometry
read
 volume

t
y
p
e
=
r
a
n
d
o
m
b
a
t
c
h
e
s
=1000
```

(continues on next page)

(continued from previous page)

```
end
 volume
read
 plot

s
c
r
=
y
e
s
l
p
i
=10

t
t
l
='y-z slice at x=0.0  through centerline of both pipes'

x
u
l
=0
.0
y
u
l
=
-39
.0
z
u
l
=137
.0

x
l
r
=0
.0
y
l
r
=105
.0
z
l
r
=
-105
.0

v
a
x
=1
w
d
n
=
```

(continues on next page)

(continued from previous page)

```
n
a
x
=400  end
 plt
0

t
t
l
='x-y slice at z=26.0  slightly above point of separation'

x
u
l
=
-40
.0
y
u
l
=105
.0
z
u
l
=26
.0

x
l
r
=
+40
.0
y
l
r
=
-40
.0
z
l
r
=26
.0

u
a
x
=1
v
d
n
=
-1
```

(continues on next page)

(continued from previous page)

```
n
a
x
=400 end
 plt
l

t
t
l
='x-y slice at z=75.0  well above point of separation'

x
u
l
=
-40
.0
y
u
l
=105
.0
z
u
l
=75
.0

x
l
r
=
+40
.0
y
l
r
=
-40
.0
z
l
r
=75
.0

u
a
x
=1
v
d
n
=
-1
```

(continues on next page)

(continued from previous page)

```
n
a
x
=400 end
 plt
2
end
 plot
end
 data
end
```

9.5.2 Sample Problem 2: Plexiglas Cross

The purpose of this problem is to calculate the k-effective of a system composed of intersecting Plexiglas pipes, in the shape of a cross, filled with a 5% enriched UO_2F_2 solution. The room temperature UO_2F_2 solution contains 896.1 gm/l of uranium, no excess acid, and has a specific gravity of 2.015 gm/cm^3. The pipes have a 13.335 cm inner diameter and 16.19 cm outer diameter. The vertical pipe is open on the top and 3.17 cm thick on the bottom. The horizontal pipe ends are 3.17 thick. The vertical pipe is 210.19 cm in length and filled with solution to a height of 117.2 cm. The two horizontal legs, positioned in the XZ-plane, intersect the vertical pipe 91.44 cm from the outside bottom at an 89 degree angle with the upper section of the pipe. Each horizontal is 91.44 cm in length and filled with the above specified UO_2F_2 solution. A water reflector surrounding the solution filled pipes extends out from the point where the pipes intersect 111.76 cm in the ±X directions, 20.64 cm in the ±Y directions, 29.03 cm in the +Z direction, and –118.428 cm in the –Z direction.

```
=csas6

s
a
m
p
l
e
p
r
o
b
l
e
m 2  89
-
c
r
o
s
s
, 5
%
u
o2
f2
s
o
l
n
,
```

(continues on next page)

```
l
e
x
i
```

Fig. 9.2: Critical assembly of UO_2F_2 solution in a Plexiglas cross.

(continued from previous page)

```
v7
-238
read
 comp

s
o
l
u
t
i
o
n

m
i
x
=1

r
h
o
[
u
o2
f2
]
=896
.1 92235 5
.0 92238 95
.0

d
e
n
s
i
t
y
=
?

t
e
m
p
e
r
a
t
u
r
e
=298
.0
  end
 solution
```

(continues on next page)

(continued from previous page)

```
p
l
e
x
i
g
l
a
s
s 3 1
.0 end

h2
o        2 1
.0 end
end
 comp
read
 param

p
l
t
=
y
e
s
end
 param
read
 geom

g
l
o
b
a
l
u
n
i
t 1

c
y
l
i
n
d
e
r  10  13
.335 28
.93
-88
.27
```

(continues on next page)

```
c
y
l
i
n
d
e
```

(continued from previous page)

```
c
y
l
i
n
d
e
r  30  16
.19 121
.92
-91
.44

c
y
l
i
n
d
e
r  40  13
.335 88
.27 0
.0
r
o
t
a
t
e
a1
=90
.
a2
=89
.

c
y
l
i
n
d
e
r  50  16
.19  91
.44 0
.0
r
o
t
a
t
e
a1
=90
.
a2
=89
.
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r  60  13
.335 88
.27 0
.0
r
o
t
a
t
e
a1
=
-90
.
a2
=89
.

c
y
l
i
n
d
e
r  70  16
.19  91
.44 0
.0
r
o
t
a
t
e
a1
=
-90
.
a2
=89
.

c
u
b
o
i
d    80  2
p111
.74 2
p20
.64 29
.03
-118
.428
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d    90  2
p111
.74 2
p40
.64 121
.92
-118
.428

m
e
d
i
a 1 1 10

m
e
d
i
a 0 1 20
-10

m
e
d
i
a 3 1 30
-10
-20
-50
-70

m
e
d
i
a 1 1 40
-10
-20

m
e
d
i
a 3 1 50
-40
-10
-20

m
e
d
i
a 1 1 60
-10
-20
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a 3 1 70
-60
-10
-20
-50

m
e
d
i
a 2 1 80
-10
-20
-30
-40
-50
-60
-70

m
e
d
i
a 0 1 90
-20
-30
-80

b
o
u
n
d
a
r
y  90
end
 geom
read
 volume

t
y
p
e
=
t
r
a
c
e
end
 volume
```

(continues on next page)

(continued from previous page)

```
read
 start

n
s
t
=6
t
f
x
=0
.
t
f
y
=0
.
t
f
z
=0
.
l
n
u
=1000
end
 start
read
 plot

s
c
r
=
y
e
s
l
p
i
=10

t
t
l
=' x-z slice at y=0.0 '

x
u
l
=
-113
.
y
u
l
```

(continues on next page)

```
=0
.
z
u
l
=  48
.
```

(continued from previous page)

```
x
l
r
= 113
.
y
l
r
=0
.
z
l
r
=
-120
.

u
a
x
=1
.0
w
d
n
=
-1
.0

n
a
x
=400  end
 plt
0

t
t
l
=' y-z slce at x=0.0 '

x
u
l
=0
.
y
u
l
=
-42
.
z
u
l
= 122
.
```

(continues on next page)

(continued from previous page)

```
x
l
r
=0
.
y
l
r
= 42
.
z
l
r
=
-120
.

v
a
x
=1
.0
w
d
n
=
-1
.0

n
a
x
=400  end
 plt
1

t
t
l
=' x-y slice at z=0.0 '

x
u
l
=
-113
.0
y
u
l
= 42
.
z
u
l
=0
.
```

(continues on next page)

(continued from previous page)

```
x
l
r
= 113
.0
y
l
r
=
-42
.
z
l
r
=0
.

u
a
x
=1
.0
v
d
n
=
-1
.0

n
a
x
=400  end
 plt
2
end
 plot
end
 data
end
```

9.5.3 Sample Problem 3: Sphere

This problem models an assembly consisting of a 93.2% enriched bare uranium sphere, 8.741 cm in radius, having a density of 18.76 gm/cm^3. Problem 3 models the assembly as a single bare sphere. The second problem models the assembly as a hemisphere with mirror reflection on the flat surface. The next three problems model the sphere using chords. This set of four problems is designed to illustrate the use of multiple chords in a problem.

```
=csas6

s
a
m
p
l
e
p
l
o
b
l
```

(continues on next page)

(continued from previous page)

```
v7
-238
read
 comp

u
r
a
n
i
u
m  1
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end
end
 comp
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

s
p
h
e
r
e 10  8
.741

c
u
b
o
i
d   20  6
p8
.741

m
e
d
i
a  1 1 10
v
o
l
=2797
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  0 1 20
-10
v
o
l
=2545
.3424

b
o
u
n
d
a
r
y 20
end
 geometry
end
 data
end
```

9.5.4 Sample Problem 4: Sphere Models Using Chords and Mirror Albedos

This problem models an assembly consisting of a 93.2% enriched bare uranium sphere, 8.741 cm in radius, having a density of 18.76 gm/cm^3. The problem models the assembly as a hemisphere with mirror reflection on the flat surface.

```
=csas6

s
a
m
p
l
e
p
r
o
b
l
e
m 4
b
a
r
e 93
.2
%
U
s
p
h
e
e
,
h
e
```

(continues on next page)

(continued from previous page)

```
v7
-238
read
 comp

u
r
a
n
i
u
m  1
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end
end
 comp
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

s
p
h
e
r
e 10  8
.741
c
h
o
r
d
+
x
=0
.0

c
u
b
o
i
d 20  6
.741 0
.0  8
.741
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  1 1 10
v
o
l
=2797
.5121

m
e
d
i
a  0 1 20
-10
v
o
l
=2545
.3424

b
o
u
n
d
a
r
y 20
end
 geometry
read
 bounds

-
x
b
=
m
i
r
r
o
r
end
 bounds
end
 data
end
```

9.5.5 Sample Problem 5: Sphere Models Using Chords and Mirror Albedos

This problem models an assembly consisting of a 93.2% enriched bare uranium sphere, 8.741 cm in radius, having a density of 18.76 gm/cm^3. The problem models the assembly as a quarter sphere with mirror reflection on the two flat surfaces.

```
=csas6

s
a
m
p
l
e
p
r
o
b
l
e
m 5
b
a
r
e 93
.2
%
U
s
p
h
e
r
e
,
q
u
a
r
t
e
r
s
p
h
e
r
e
w
/
m
i
r
r
o
r
a
l
b
e
d
```

(continues on next page)

(continued from previous page)

```
v7
-238
read
 comp

u
r
a
n
i
u
m  1
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end
end
 comp
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

s
p
h
e
r
e 10  8
.741
c
h
o
r
d
+
x
=0
.0
c
h
o
r
d
+
y
=0
.0
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d   20  8
.741 0
.0 8
.741 0
.0 8
.741
-8
.741

m
e
d
i
a  1 1 10
v
o
l
=2797
.5121

m
e
d
i
a  0 1 20
-10
v
o
l
=2545
.3424

b
o
u
n
d
a
r
y 20
end
 geometry
read
 bounds

-
x
y
=
m
i
r
r
o
r
```

(continues on next page)

(continued from previous page)

```
end
 bounds
end
 data
end
```

9.5.6 Sample Problem 6: Sphere Models Using Chords and Mirror Albedos (Eighth Sphere)

This problem models an assembly consisting of a 93.2% enriched bare uranium sphere, 8.741 cm in radius, having a density of 18.76 gm/cm^3. The problem models the assembly as an eighth sphere with mirror reflection on the three flat surfaces.

```
=csas6

s
a
m
p
l
e
p
r
o
b
l
e
m 6
b
a
r
e 93
.2
%
U
s
p
h
e
r
e
,
e
i
g
h
t
h
s
p
h
e
r
e
w
```

(continues on next page)

```
/
m
i
r
r
o
r
```

(continued from previous page)

```
v7
-238
read
 comp

u
r
a
n
i
u
m  1
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end
end
 comp
read
 geometry

g
l
o
b
a
l
u
n
i
t 1

s
p
h
e
r
e 10  8
.741
c
h
o
r
d
+
x
=0
.0
c
h
o
r
d
+
y
=0
.0
c
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d   20  8
.741 0
.0 8
.741 0
.0 8
.741 0
.0

m
e
d
i
a  1 1 10
v
o
l
=2797
.5121

m
e
d
i
a  0 1 20
-10
v
o
l
=2545
.3424

b
o
u
n
d
a
r
y 20
end
 geometry
read
 bounds

-
f
c
=
m
i
r
r
o
r
```

(continues on next page)

(continued from previous page)

```
end
 bounds
end
 data
end
```

9.5.7 Sample Problem 7: Grotesque without the Diaphragm

The purpose of this problem is to calculate the k_{eff} of a system composed of eight enriched uranium units placed on a diaphragm, with an irregularly shaped centerpiece positioned in the center hole of the diaphragm [Mih99] The assembly and centerpiece are shown in Fig. 9.3, which is Fig. 4 from Ref. 1. The eight units consist of an approximate parallelepiped with an irregular top, a parallelepiped, and six cylinders of various sizes. The centerpiece, which penetrates the hole in the diaphragm, consists of a cylinder topped by a parallelepiped topped by a hemisphere. The diaphragm is not modeled in this example.

Fig. 9.3: Grotesque experimental setup.

```
=csas6

s
a
m
p
l
e
p
r
o
b
l
e
m 7
k
e
n
o
-
v
i
```

(continues on next page)

(continued from previous page)

```
v7
-238
read
 comp

u
r
a
n
i
u
m   1
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

u
r
a
n
i
u
m   2
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

u
r
a
n
i
u
m   3
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end
```

(continues on next page)

```
u
r
a
n
i
u
m   4
```

(continued from previous page)

```
u
r
a
n
i
u
m   5
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

u
r
a
n
i
u
m   6
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

u
r
a
n
i
u
m   7
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

u
r
a
n
i
u
m   8
d
e
n
=18
.76 1 293 92235 93
```

(continues on next page)

(continued from previous page)

```
u
r
a
n
i
u
m   9
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

u
r
a
n
i
u
m  10
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

u
r
a
n
i
u
m  11
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

u
r
a
n
i
u
m  12
d
e
n
=18
.76 1 293 92235 93
```

(continues on next page)

(continued from previous page)

```
u
r
a
n
i
u
m  13
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end

u
r
a
n
i
u
m  14
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end
end
 comp
read
 param

p
g
m
=
y
e
s
p
l
t
=
y
e
s
end
 param
read
 geom
```

(continues on next page)

(continued from previous page)

```
g
l
o
b
a
l
u
n
i
t 1
'*** one through three is item 1 in drawing 84-10649 ornl/csd/tm-220 ***
'one    top piece of item 1

c
u
b
o
i
d 10  2
p6
.3515 1
.2685
-3
.8115 13
.377 13
.058
o
r
i
g
i
n
y
=
-17
.464
z
=0
.15
r
o
t
a
t
e
a2
=
-1
.35
'two    middle piece of item 1

c
u
b
o
i
d 20  2
p6
.3515 6
.3515
-3
.8115 13
.058 11
```

(continues on next page)

(continued from previous page)

```
'three  bottom piece of item 1

c
u
b
o
i
d 30  4
p6
.3515 11
.155 0
.
o
r
i
g
i
n
y
=
-17
.464
z
=0
.15
r
o
t
a
t
e
a2
=
-1
.35
'*** four is item 2 in drawing 84-10649 ornl/csd/tm-220 ***

c
y
l
i
n
d
e
r 40 4
.555 12
.918 0
.
o
r
i
g
i
n
x
=
-12
.176
y
=
-9
.343
z
=0
```

(continues on next page)

(continued from previous page)

```
'*** five is item 3 in drawing 84-10649 ornl/csd/tm-220 ***

c
y
l
i
n
d
e
r 50 5
.761 13
.475 0
.
o
r
i
g
i
n
x
=
-16
.333
y
=1
.681
z
=0
.174
r
o
t
a
t
e
a1
=83
.5
a2
=
+1
.173
'*** six is item 4 in drawing 84-10649 ornl/csd/tm-220 ***

c
y
l
i
n
d
e
r 60 4
.5525 12
.969 0
.
o
r
i
g
i
n
x
=
-9
```

(continues on next page)

(continued from previous page)

```
'*** seven and eight are item 5 in drawing 84-10649 ornl/csd/tm-220 ***
'seven

c
u
b
o
i
d  70  2
p3
.81 8
.13
-4
.573 8
.91 0
.
o
r
i
g
i
n
y
=15
.698
z
=0
.290
r
o
t
a
t
e
a2
=
+2
.58
'eight

c
y
l
i
n
d
e
r 80 4
.573 13
.229 8
.91
o
r
i
g
i
n
y
=15
.698
z
=0
.290
r
```

(continues on next page)

(continued from previous page)

```
'*** nine is item 6 in drawing 84-10649 ornl/csd/tm-220 ***

c
y
l
i
n
d
e
r 90 4
.5545 12
.974 0
.
o
r
i
g
i
n
x
=9
.854
y
=10
.964
z
=0
.134
r
o
t
a
t
e
a1
=
-42
.0
a2
=
+1
.680
'*** ten is item 7 in drawing 84-10649 ornl/csd/tm-220 ***

c
y
l
i
n
d
e
r 100 5
.7495 13
.475 0
.
o
r
i
g
i
n
x
=16
.388
```

(continues on next page)

(continued from previous page)

```
'*** eleven is item 8 in drawing 84-10649 ornl/csd/tm-220 ***

c
y
l
i
n
d
e
r 110 4
.5565 12
.954 0
.
o
r
i
g
i
n
x
=12
.029
y
=
-9
.398
z
=0
.087
r
o
t
a
t
e
a1
=38
.0
a2
=
-1
.100
'*12 through 14 is the centerpiece in drawing 84-10649 ornl/csd/tm-220
'twelve

c
y
l
i
n
d
e
r 120 5
.757 2
.690 0
.
o
r
i
g
i
n
x
=
```

(continues on next page)

(continued from previous page)

```
'thirteen

c
u
b
o
i
d 130 4
p6
.35 5
.718 0
.
o
r
i
g
i
n
z
=0
.937
'fourteen

s
p
h
e
r
e    140 6
.082
c
h
o
r
d
+
z
=0
.
o
r
i
g
i
n
x
=
-0
.268
y
=0
.268
z
=6
.655
'*** fifteen is the system boundary ***
'fifteen
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d   150 4
p25
.0 15
.0
-2
.0

m
e
d
i
a  1 1
+10
v
o
l
=20
.58546556

m
e
d
i
a  2 1
+20
-10
v
o
l
=245
.678420867

m
e
d
i
a  3 1
+30
-20
v
o
l
=1800
.040061395

m
e
d
i
a  4 1
+40
v
o
l
=842
.019046637
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a  5 1
+50
v
o
l
=1404
.99376489

m
e
d
i
a  6 1
+60
v
o
l
=844
.415646269

m
e
d
i
a  7 1
+70
v
o
l
=862
.4600226

m
e
d
i
a  8 1
+80
-70
v
o
l
=283
.749744681

m
e
d
i
a  9 1
+90
v
o
l
=845
.485582679
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a 10 1
+100
v
o
l
=1399
.390119093

m
e
d
i
a 11 1
+110
v
o
l
=844
.921798001

m
e
d
i
a 12 1
+120
-130
v
o
l
=280
.088070346

m
e
d
i
a 13 1
+130
v
o
l
=922
.25622

m
e
d
i
a 14 1
+140
-130
v
o
l
=471
.191948666
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a 0 1 150
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100

-110
-120
-130
-140
v
o
l
=31432
.726088316

b
o
u
n
d
a
r
y 150
end
 geom
read
 plot

s
c
r
=
y
e
s
l
p
i
=10

c
l
r
= 1 255   0   0
                2   0   0 205
```

(continues on next page)

(continued from previous page)

```
                 3    0 229 238
                 4    0 238   0
                 5  205 205   0
                 6  255 121 121
                 7  145  44 238
                 8  150 150 150
                 9  240 200 220
                10    0 191 255
                11  224 255 255
                12    0 128  64
                13  255 202 149
                14  255   0 128
             end
 color

t
t
l
='grotesque x-y slice at z=0.5'

x
u
l
=
-25
.5
y
u
l
= 25
.5
z
u
l
=0
.5

x
l
r
= 25
.5
y
l
r
=
-25
.5
z
l
r
=
.5

u
a
x
=1
v
d
n
=
-1
n
```

(continues on next page)

(continued from previous page)

```
t
t
l
='grotesque x-y slice at z=2.0'

x
u
l
=
-25
.5
y
u
l
= 25
.5
z
u
l
=2

x
l
r
= 25
.5
y
l
r
=
-25
.5
z
l
r
=2 end

t
t
l
='grotesque x-y slice at z=9.5'

x
u
l
=
-25
.5
y
u
l
= 25
.5
z
u
l
```

(continues on next page)

```
=9
.5
```

(continued from previous page)

```
x
l
r
= 25
.5
y
l
r
=
-25
.5
z
l
r
=9
.5 end

t
t
l
='grotesque y-z slice at x=-0.593'

x
u
l
=
-
.593
y
u
l
=
-25
.5
z
u
l
=15
.5

x
l
r
=
-
.593
y
l
r
= 25
.5
z
l
r
=
-3
.5
```

(continues on next page)

(continued from previous page)

```
u
a
x
=0
v
a
x
=1

v
d
n
=0
w
d
n
=
-1
n
a
x
=800  end

t
t
l
='grotesque x-z slice at y=0.0'

x
u
l
=
-25
.5
y
u
l
=0
.0
z
u
l
=15
.5

x
l
r
= 25
.5
y
l
r
=0
.0
z
l
r
=
5
.5
```

(continues on next page)

(continued from previous page)

```
u
a
x
=1
v
a
x
=0
w
a
x
=0

u
d
n
=0
v
d
n
=0
w
d
n
=
-1
n
a
x
=800  end

t
t
l
='grotesque x-z slice at y=12.125'

x
u
l
=
-25
.5
y
u
l
=12
.125
z
u
l
=15
.5

x
l
r
= 25
.5
y
l
r
=12
.125
```

(continues on next page)

(continued from previous page)

```
u
a
x
=1
v
a
x
=0
w
a
x
=0

u
d
n
=0
v
d
n
=0
w
d
n
=
-1
n
a
x
=800  end

t
t
l
='grotesque x-z slice at y=-12.000'

x
u
l
=
-25
.5
y
u
l
=
-12
.000
z
u
l
=15
.5

x
l
r
= 25
.5
y
l
r
=
```

(continues on next page)

(continued from previous page)

```
u
a
x
=1
v
a
x
=0
w
a
x
=0

u
d
n
=0
v
d
n
=0
w
d
n
=
-1
n
a
x
=800  end
end
 plot
end
 data
end
```

9.5.8 Sample Problem 8 Infinite Array of MOX and UO2 Assemblies

The purpose of this problem is to calculate the *keff* of a system composed of an infinite array of MOX assemblies interspersed between UO_2 assemblies. Both assembly types contain 331 pins in a hexagonal lattice with a pin pitch of 1.275 cm and an assembly pitch of 23.60 cm as shown in Fig. 9.4. The moderator is borated water at 306°C having a density of 0.71533 gm/cc and composed of 99.94 wt % H_2O and 0.06 wt % natural boron. Each fuel rod is 355 cm in length, has a radius of 0.3860 cm, 0.722-cm-thick Zr cladding with no gap, and is at a temperature of 754°C.

The UO_2 fuel consists of 4.4 wt % ^{235}U and 95.6 wt % ^{238}U at a density of 8.7922 gm/cc. The UO_2 fuel also contains 9.4581E–9 atoms/b-cm of ^{135}Xe and 7.3667E–8 atoms/b-cm of ^{149}Sm.

The MOX fuel consists of 96.38 wt % UO_2 and 3.62 wt % PuO_2 at a density of 8.8182 gm/cc. The UO_2 fuel is composed of 2.0 wt % ^{235}U and 98.0 wt % ^{238}U. The PuO_2 fuel is composed of 93.0 wt % ^{239}Pu, 6.0 wt % ^{240}Pu- and 1.0 wt % ^{241}Pu. The MOX fuel also contains 9.4581E–9 atoms/b-cm of ^{135}Xe and 7.3667E–8 atoms/b-cm of ^{149}Sm.

These two assemblies are placed so they represent an infinite array in the X and Y dimensions as shown in Fig. 9.5. There is 20 cm of water above and below fuel assemblies. This problem uses CENTRM/PMC as the resolved resonance processor cross section. Since an infinite array cannot be explicitly modeled, a section of the array is modeled and the X and Y sides have mirror reflection.

```
=csas6        parm=(centrm)

s
a
m
p
l
e
p
r
o
b
l
e
m 8
-
V
V
E
R
i
n
f
.
a
r
r
a
y
-
M
O
X
&
U
O2
A
s
s
e
m
b
l
i
e
s

v7
-238
read
 comp
'  UO2 Fuel

u
o2      1
d
e
n
=8
.7922 1
 0 1027 92235 4
.4  92238 95
.6 end
```

(continues on next page)

(continued from previous page)

```
x
e
-135  1 0 9
.4581
E
-09 1027 end

s
m
-149  1 0 7
.3667
E
-08 1027 end
'  MOX Fuel

u
o2     2
d
e
n
=8
.8182 0
.9638 1027  92235  2
.0 92238 98
.0 end

p
u
o2    2
d
e
n
=8
.8182 0
.0362 1027  94239 93
.0 94240  6
.0 94241  1
.0 end

x
e
-135  2 0 9
.4581
E
-09 1027 end

s
m
-149  2 0 7
.3667
E
-08 1027 end
'  Cladding for UO2 fuel

z
r      3
d
e
n
=6
.4073 1
.0  579  end
```

(continues on next page)

(continued from previous page)

```
'  Moderator for UO2 fuel

h2
o     4
d
e
n
=0
.71533 0
.9994 579 end

b
o
r
o
n   4
d
e
n
=0
.71533 0
.0006 579 end
'  Cladding for MOX fuel

z
r      5
d
e
n
=6
.4073 1
.0  579  end
'  Moderator for MOX fuel

h2
o     6
d
e
n
=0
.71533 0
.9994 579 end

b
o
r
o
n   6
d
e
n
=0
.71533 0
.0006 579 end
'  Moderator for vacant units

h2
o     7
d
e
n
=0
.71533 0
.9994 579 end
```

(continues on next page)

(continued from previous page)

```
b
o
r
o
n   7
d
e
n
=0
.71533 0
.0006 579 end
end
 comp
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
t
r
i
a
n
g
p
i
t
c
h
p
i
t
c
h
=1
.2750 4
f
u
e
l
d
=0
.7720 1
c
l
a
d
d
=0
.9164 3 end
```

(continues on next page)

(continued from previous page)

```
l
a
t
t
i
c
e
c
e
l
l
t
r
i
a
n
g
p
i
t
c
h
p
i
t
c
h
=1
.2750 6
f
u
e
l
d
=0
.7720 2
c
l
a
d
d
=0
.9164 5 end
'  more data  dab=500  end more
end
 celldata
read
 param

g
e
n
=203
n
p
g
=1000
```

(continues on next page)

(continued from previous page)

```
end
 param
read
 bounds

a
l
l
=
m
i
r
r
o
r
z
f
c
=
v
o
i
d
end
 bounds
read
 geom

u
n
i
t   1

c
o
m
='UO2 Fuel Rod'

c
y
l
i
n
d
e
r 10 0
.3860 355
.0 0
.0

c
y
l
i
n
d
e
r 20 0
.4582 355
.0 0
.0
```

(continues on next page)

(continued from previous page)

```
h
e
x
p
r
i
s
m 30 0
.6375 355
.0 0
.0

m
e
d
i
a 1 1 10

m
e
d
i
a 3 1 20
-10

m
e
d
i
a 4 1 30
-20

b
o
u
n
d
a
r
y 30

u
n
i
t  2

c
o
m
='Vacant(water filled) hex'

h
e
x
p
r
i
s
m 10 0
.6375 355
.0 0
.0
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a 7 1 10

b
o
u
n
d
a
r
y 10

u
n
i
t  3

c
o
m
='Vacant(water filled) hex'

h
e
x
p
r
i
s
m 10 0
.6375 355
.0 0
.0

m
e
d
i
a 7 1 10

b
o
u
n
d
a
r
y 10

u
n
i
t   4
```

(continues on next page)

(continued from previous page)

```
c
o
m
='MOX Fuel Rod'

c
y
l
i
n
d
e
r 10 0
.3860 355
.0 0
.0

c
y
l
i
n
d
e
r 20 0
.4582 355
.0 0
.0

h
e
x
p
r
i
s
m 30 0
.6375 355
.0 0
.0

m
e
d
i
a 2 1 10

m
e
d
i
a 5 1 20
-10

m
e
d
i
a 6 1 30
-20
```

(continues on next page)

(continued from previous page)

```
b
o
u
n
d
a
r
y 30

g
l
o
b
a
l
u
n
i
t 5

r
h
e
x
p
r
i
s
m 10 11
.800 355
.0 0
.0

r
h
e
x
p
r
i
s
m 20 11
.800 355
.0 0
.0
o
r
i
g
i
n
y
=23
.6

r
h
e
x
p
r
i
s
```

(continues on next page)

(continued from previous page)

```
r
h
e
x
p
r
i
s
m 40 11
.800 355
.0 0
.0
o
r
i
g
i
n
x
=20
.4382
y
=35
.4

c
u
b
o
i
d   50 20
.4382 0
.0 35
.4 0
.0 375
.0
-20
.0

a
r
r
a
y 1  10
-20
-30
-40
p
l
a
c
e 12 12 1  0
.0       0
.0  0
.0
```

(continues on next page)

```
a
r
r
a
y 2  20
-10
-30
```

(continued from previous page)

```
a
r
r
a
y 2  30
-10
-20
-40
p
l
a
c
e 12 12 1  20
.4382  11
.8  0
.0

a
r
r
a
y 1  40
-10
-20
-30
p
l
a
c
e 12 12 1  20
.4382  35
.4  0
.0

m
e
d
i
a 4 1 50
-10
-20
-30
-40

b
o
u
n
d
a
r
y 50
end
 geom
read
 array
```

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```
a
r
a
=1
t
y
p
=
s
h
e
x
a
g
o
n
a
l
n
u
x
=23
n
u
y
=23
n
u
z
=1

f
i
l
l
   3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
    3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3 3 3
   3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3 3
    3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3 3
   3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3
    3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3
   3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3
    3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3
   3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3
    3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3
   3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3
    3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3
   3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3
    3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3
   3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3
    3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3
   3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3
    3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3
   3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3 3
    3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3 3
   3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3 3
```

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```
    3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 3 3 3 3 3 3
   3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
    end
 fill

a
r
a
=2
t
y
p
=
s
h
e
x
a
g
o
n
a
l
n
u
x
=23
n
u
y
=23
n
u
z
=1

f
i
l
l
   2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
    2 2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2
   2 2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2
    2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2
   2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2
    2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2
   2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2
    2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2
   2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2
    2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2
   2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2
    2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2
   2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2
    2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2
   2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2
    2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2
   2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2
```

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```
    2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2
   2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2
    2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2
   2 2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2
    2 2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2
   2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
    end
 fill
end
 array
read
 plot

l
p
i
=10
s
c
r
=
y
e
s

t
t
l
='VVER assembly x-y x-section'

x
u
l
=
-0
.1
y
u
l
=35
.5
z
u
l
=10

x
l
r
=20
.6
y
l
r
=
-0
.1
z
l
r
=10
```

(continues on next page)

(continued from previous page)

```
u
a
x
=1
v
d
n
=
-1
.0

n
a
x
=640
p
i
c
=
m
a
t   end
 plt
1
end
 plot
read
 volume

t
y
p
e
=
r
a
n
d
o
m
b
a
t
c
h
e
s
=1000
end
 volume
end
 data
end
```

Fig. 9.4: MOX or UO_2 hexagonal assembly.

Fig. 9.5: Infinite array of MOX assemblies interspersed between UO_2 assemblies.

9.6 Warning and Error Messages

CSAS6 contains two types of warning and error messages. The first type of message is from XSProc is common to many of the SCALE analytical sequences. The second type of message is from the CSAS6 subroutines and is identified by CS- followed by a number. These messages are listed in numerical order below. For additional information concerning a message, simply look up the number in this section.

Warning messages appear when a possible error is encountered. It is the responsibility of the user to verify whether the data are correct when a warning message is encountered. The functional modules activated by CSAS6 and related sequences will be executed even though a warning message has been generated.

When an error is recognized, an error message is written and an error flag is set so the functional modules will not be activated. The code stops immediately if the error is too severe to allow continuation of input. However, it will continue to read and check the data if it is able. When the data reading is completed, execution is terminated if an error flag was set when the data were being processed. If the error flag has not been set, execution continues. When error messages are printed, the user should focus on the first error message, because subsequent messages may have been caused by the error that generated the first message.

The following messages originate in the part of CSAS6 that reads, checks, and prepares data for KENO-VI. The same set of error messages are also used for CSAS5 that reads, checks, and prepares data for KENO V.a and MODIFY. CSAS6 is not capable of performing searches at this time. An error message referring to a SEARCH routine, from a CSAS6 problem, indicates a code error.

CS-16 ***WARNING* READ FLAG NOT FOUND. ASSUME KENO V PARAMETER DATA FOLLOWS.** This message from subroutine CPARAM indicates that the word READ is not the first word of KENO-VI data following the Material Information Processor input data. If parameter data is to be entered, the code expects the words READ PARAMETERS to precede the parameter input data. If the word READ is not the first word, the code assumes the data are parameter input data.

CS-21 A UNIT NUMBER WAS ENTERED FOR THE CROSS-SECTION LIBRARY. (LIB= IN PARAMETER DATA.) THE D This message is from subroutine CPARAM. It indicates that a value has been entered for the cross-section library in the KENO-VI parameter data. The cross-section library created by the analytical sequence should be used. MAKE CERTAIN THAT THE CORRECT CROSS SECTIONS ARE BEING USED.

CS-55 * ERRORS WERE ENCOUNTERED IN PROCESSING THE CSAS-KENO6 DATA. EXECUTION IS IMPOSSIBLE** This message from subroutine SASSY is printed if errors were found in the KENO-VI input data for CSAS. If a search is being made, data reading will continue until all the data have been entered or a fatal error terminates the data reading. When the data reading and checking have been completed, the problem will terminate without executing. Check the printout to locate the errors responsible for this message.

CS-62 * ERROR *** MIXTURE _____ IN THE GEOMETRY WAS NOT CREATED IN THE STANDARD COMPOSITIO** This message from subroutine MIXCHK indicates that a mixture specified in the KENO-VI geometry was not created in the standard composition data.

CS-68 * ERROR *** AN INPUT DATA ERROR HAS BEEN ENCOUNTERED IN THE DATA ENTERED FOR THIS PRO** This message from the main program, CSAS6, is printed if the subroutine library routine LRDERR returns a value of "TRUE," indicating that a reading error has been encountered in the "KENO PARAMETER" data. The appropriate data type is printed in the message. Locate the unnumbered message stating "*** **ERROR IN INPUT. CARD IMAGE PRINTED ON NEXT LINE** ***." Correct the data and resubmit the problem.

CS-69 ***ERROR* MIXTURE _____ IS AN INAPPROPRIATE MIXTURE NUMBER FOR USE IN THE KENO GEOM** This message from subroutine CMXCHK indicates that a mixture that is a component of a cell-weighted mixture has been used in the KENO-VI geometry data.

CS-82 * AN ERROR WAS ENCOUNTERED IN ONE OF THE FUNCTIONAL MODULES.** This message from CSAS6 indicates that an error was encountered during execution of one of the functional modules such as CRAWDAD, BONAMI, CENTRM, PMC, XSDRNPM, or KENO-VI. Check the printout to locate and correct the error.

CS-99 THIS PROBLEM WILL NOT BE RUN BECAUSE PARM=CHECK WAS ENTERED IN THE ANALYTICAL SEQUEN

This message from subroutine CSAS indicates that the problem data were read and checked and no errors were found. To execute the problem, remove the PARM=CHECK or PARM=CHK from the analytical sequence indicator data entry.

CS-100 THIS PROBLEM WILL NOT BE RUN BECAUSE ERRORS WERE ENCOUNTERED IN THE INPUT DATA.

This message from subroutine CSAS is self-explanatory. Examine the printout to locate the error or errors in the input data. Correct them and resubmit the problem.

CHAPTER

TEN

ADDITIONAL EXAMPLE APPLICATIONS OF CSAS6

Several example uses of CSAS6 are shown in this section for a variety of applications.

10.1 Run KENO-VI using CSAS6

CSAS6 creates a microscopic working format library and a mixing table that is passed to KENO-VI. The library is created using CENTRM/PMC/WORKER to process the cross section data in the resolved resonance regions of the isotopes contained in the library. CSAS6 then executes KENO-VI, which calculates k_{eff} for the problem. The following examples are for using the multigroup mode of calculation for KENO-VI. Using the continuous energy mode can be accomplished by simply changing the library name to one of the continuous energy libraries.

EXAMPLE 1. CSAS6 – Determine the k_{eff} of a system.

Consider a problem consisting of eight uranium metal cylinders that are 93.2% wt enriched, having a density of 18.76 g/cm^3. The cylinders are arranged in a $2 \times 2 \times 2$ array. Each has a radius of 5.748 cm and a height of 10.765 cm. The center-to-center spacing in the horizontal (X-Y) plane is 13.74 cm and the vertical center-to-center spacing is 13.01 cm. Because the cross section processing will be done assuming an infinite homogeneous medium and no cell mixtures are used, there is no unit cell data. The input data for this problem follow.

```
=CSAS6

S
E
T
U
P 2
C8
I
N
C
S
A
S6

V7
-238

R
E
A
D
C
O
M
P
```

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(continued from previous page)

```
U
R
A
N
I
U
M  1
D
E
N
=18
.76 1 293  92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2
E
N
D

E
N
D
C
O
M
P

R
E
A
D
P
A
R
A
M
E
T
E
R
S
F
L
X
=
Y
E
S
F
D
N
=
Y
E
S
F
A
R
=
Y
E
S
=
```

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(continued from previous page)

```
R
E
A
D
G
E
O
M
E
T
R
Y

U
N
I
T 1

C
Y
L
I
N
D
E
R 10  5
.748 5
.3825
-5
.3825

C
U
B
O
I
D   20  6
.87
-6
.87 6
.87
-6
.87 6
.505
-6
.505

M
E
D
I
A 1 1 10

M
E
D
I
A 0 1 20
-10
```

(continues on next page)

(continued from previous page)

```
B
O
U
N
D
A
R
Y 20

G
L
O
B
A
L
U
N
I
T 2

C
U
B
O
I
D 10 4
P13
.74   2
P13
.010

A
R
R
A
Y  1  10
P
L
A
C
E 1 1 1
-6
.87
-6
.87
-6
.505

B
O
U
N
D
A
R
Y 10
```

(continues on next page)

(continued from previous page)

```
E
N
D
G
E
O
M
E
T
R
Y

R
E
A
D
A
R
R
A
Y

G
B
L
=1
A
R
A
=1
N
U
X
=2
N
U
Y
=2
N
U
Z
=2
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y
```

(continues on next page)

(continued from previous page)

```
E
N
D
D
A
T
A

E
N
D
```

EXAMPLE 2. CSAS6 – Determine the k_{eff} of an array of fuel pellets in a UO_2F_2 solution.

Consider a 60 cm inside diameter cylindrical tank filled with 5.0%-enriched UO_2 fuel rods and 5.0%-enriched UO_2F_2 solution at 295 gm/liter. A 51 × 51 × 1 array of fuel rods is centered on the bottom of the tank. The fuel rods are 366 cm long, 0.45 cm in radius, clad with 0.01-cm-thick Al, and at a pitch of 1.5 cm. The fuel rods sit on the bottom of the container and the container and solution rise 5.0 cm above the top of the rods. The container is 10 cm thick in the side and bottom and open at the top. Determine the k_{eff} of the system. Input data for this problem follow.

```
=CSAS6

U
O2
p
i
n
s
i
n
a
U
O2
F2
s
o
l
u
t
i
o
n

V7
-238

R
E
A
D
C
O
M
P

U
O2        1 0
.95 300 92235 5
.0 92238 95
.0
E
N
D
```

(continues on next page)

(continued from previous page)

```
A
L         2 1
.0  300
E
N
D

S
O
L
N
U
O2
F2 3 295 0
.0 1
.0 300 92235 5
.0 92238 95
.0
E
N
D

A
L         4 1
.0  300
E
N
D

S
O
L
N
U
O2
F2 5 295 0
.0 1
.0 300 92235 5
.0 92238 95
.0
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
```

(continues on next page)

(continued from previous page)

```
L
A
T
T
I
C
E
C
E
L
L
S
Q
U
A
R
E
P
I
T
C
H
P
I
T
C
H
=1
.50 3
F
U
E
L
D
=0
.9  1
C
L
A
D
D
=0
.94 2
E
N
D

E
N
D
C
E
L
L
D
A
T
A
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
G
E
O
M

U
N
I
T  1

C
O
M
='FUEL PIN'

C
Y
L
I
N
D
E
R 10  0
.45  2
P183
.0

C
Y
L
I
N
D
E
R 20  0
.47 2
P183
.1

C
U
B
O
I
D     30  4
P0
.75 2
P183
.1

M
E
D
I
A 1 1 10
```

(continues on next page)

(continued from previous page)

```
M
E
D
I
A 2 1 20
-10

M
E
D
I
A 3 1 30
-20
-10

B
O
U
N
D
A
R
Y 30

G
L
O
B
A
L
U
N
I
T  2

C
O
M
='FUEL PINS AND SOLUTION IN TANK'

C
U
B
O
I
D    10  4
P38
.25  2
P183
.1

C
Y
L
I
N
D
E
R  20  60
.0 188
.1
-183
.1
```

(continues on next page)

(continued from previous page)

```
C
Y
L
I
N
D
E
R  30  70
.0  188
.1
-193
.1

A
R
R
A
Y  1  10
P
L
A
C
E 26 26 1 3
*0
.0

M
E
D
I
A  5  1  20
-10

M
E
D
I
A  4  1  30
-20

B
O
U
N
D
A
R
Y  30

E
N
D
G
E
O
M
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=51
N
U
Y
=51
N
U
Z
=1
F
I
L
L
F1
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

E
N
D
D
A
T
A

E
N
D
```

(continues on next page)

(continued from previous page)

10.2 Run KENO-VI containing cell-weighted mixtures

CSAS6 creates a microscopic working format library and a mixing table that is passed to KENO-VI. The microscopic cross sections of the nuclides used in the unit cell geometry description are cell-weighted by specifying CELLMIX= followed by a unique mixture number. This mixture number utilizes the cell-weighted cross sections that represent the heterogeneous system. CSAS6 executes KENO-VI and calculates k_{eff} for the problem.

EXAMPLE 1. CSAS6 – Calculate the k_{eff} of an array of fuel assemblies using cell-weighted cross sections.

Consider the 4 × 4 × 1 array of fuel assemblies in a square aluminum cask described in Sect. 2.2.A.1.1, Example 2. Calculate the k_{eff} of the system by using the cell-weighted mixture 200 to represent the fuel pins in the fuel assembly. Note that mixtures 1, 2, and 3, representing UO_2, zirconium, and water, respectively, are used in the unit cell description. Cell-weighting is applied to the microscopic cross sections that are used in the cell, making them incorrect for use elsewhere. Because water is used both inside the cell and between the fuel assemblies, an additional mixture, mixture 6, has been added to represent the water between the fuel assemblies. The input data for this problem follow.

```
=CSAS6

S
Q
U
A
R
E
F
U
E
L
C
A
S
K
E
X
A
M
P
L
E
U
S
I
N
G
H
O
M
O
G
E
N
E
O
U
S
M
O
C
K
U
```

(continues on next page)

(continued from previous page)

```
V7
-238

R
E
A
D
C
O
M
P

U
O2  1
D
E
N
=9
.21 1
.0 293
. 92235 2
.35 92238 97
.65
E
N
D

Z
R   2 1
E
N
D

H2
O  3 1
E
N
D

B4
C  4 0
.367
E
N
D

A
L   4 0
.636
E
N
D

A
L   5 1
E
N
D
```

(continues on next page)

(continued from previous page)

```
H2
O   6 1
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
Q
U
A
R
E
P
I
T
C
H
P
I
T
C
H
=1
.3 3
```

(continues on next page)

```
F
U
E
L
D
=0
.8 1
```

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
P
A
R
A
M
F
A
R
=
Y
E
S
G
E
N
=253
E
N
D
P
A
R
A
M

R
E
A
D
G
E
O
M

U
N
I
T  2

C
O
M
='FUEL ASSEMBLY'
```

(continues on next page)

(continued from previous page)

```
C
U
B
O
I
D  10 4
P11
.05  2
P183
.07

C
U
B
O
I
D  20 4
P11
.70  2
P183
.72

C
U
B
O
I
D  30 4
P12
.20  2
P184
.22

M
E
D
I
A  200  1  10

M
E
D
I
A  4  1  20
-10

M
E
D
I
A  6  1  30
-20
-10

B
O
U
N
D
A
R
Y  30
```

(continues on next page)

(continued from previous page)

```
G
L
O
B
A
L
U
N
I
T 3

C
O
M
='FUEL CASK CONTAINING 4X4 ARRAY OF ASSEMBLIES'

C
U
B
O
I
D  10  4
P48
.8  2
P184
.22

C
U
B
O
I
D  20  4
P58
.8  2
P194
.22

A
R
R
A
Y  1 10
P
L
A
C
E 1 1 1
-36
.6
-36
.6 0
.0

M
E
D
I
A  5  1  20
10
```

(continues on next page)

(continued from previous page)

```
B
O
U
N
D
A
R
Y   20

E
N
D
G
E
O
M

R
E
A
D
A
R
R
A
Y

A
R
A
=1
N
U
X
=4
N
U
Y
=4
N
U
Z
=1
F
I
L
L
F2
E
N
D
F
I
L
L

E
N
D
A
R
R
A
```

(continues on next page)

(continued from previous page)

```
E
N
D
D
A
T
A

E
N
D
```

EXAMPLE 2. CSAS6 – Determine the k_{eff} of an array of fuel pellets in a UO_2F_2 solution using cell-weighted cross sections.

This is the same problem as described in *Run KENO-VI using CSAS6* Example 2. However, the rods and solutions have been replaced with a cell-weighted mixture 50. Determine the k_{eff} of the container. Input data for this problem follow.

```
=CSAS6

U
O2
p
i
n
s
i
n
a
U
O2
F2
s
o
l
u
t
i
o
n
,
c
e
l
l
-
w
e
i
g
h
t
e
d
m
i
x
t
u
r
e
```

(continues on next page)

(continued from previous page)

```
V7
-238

R
E
A
D
C
O
M
P

U
O2        1 0
.95 300 92235 5
.0 92238 95
.0
E
N
D

A
L         2 1
.0  300
E
N
D

S
O
L
N
U
O2
F2 3 295 0
.0 1
.0 300 92235 5
.0 92238 95
.0
E
N
D

A
L         4 1
.0  300
E
N
D

S
O
L
N
U
O2
F2 5 295 0
.0 1
.0 300 92235 5
.0 92238 95
.0
E
N
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
Q
U
A
R
E
P
I
T
C
H
P
I
T
C
H
=1
.50 3
F
U
E
L
D
=0
.9 1
C
L
A
D
D
=0
```

(continues on next page)

(continued from previous page)

```
E
N
D
C
E
L
L
D
A
T
A

R
E
A
D
G
E
O
M

G
L
O
B
A
L
U
N
I
T  2

C
O
M
='FUEL PINS AND SOLUTION IN TANK'

C
U
B
O
I
D    10  4
P38
.25  2
P183
.1

C
Y
L
I
N
D
E
R  20  60
.0  188
.1
=183
.1
```

(continues on next page)

(continued from previous page)

```
C
Y
L
I
N
D
E
R  30  70
.0  188
.1
-193
.1

M
E
D
I
A 50  1  10

M
E
D
I
A  5  1  20
-10

M
E
D
I
A  4  1  30
-20

B
O
U
N
D
A
R
Y  30

E
N
D
G
E
O
M

E
N
D
D
A
T
A
```

(continues on next page)

(continued from previous page)

```
E
N
D
```

10.3 Run KENO-VI containing multiple unit cells

CSAS6 can create a microscopic working format library and a mixing table that contains more than one unit cell. Each unit cell is explicitly defined in the CELLDATA section of the standard composition data. Materials may appear in only one unit cell. All materials in the standard composition that are not contained in a unit cell are processed assuming infinite homogeneous media. CSAS6 passes the created working library to KENO-VI which calculates k_{eff} for the problem.

EXAMPLE 1. CSAS6 – Calculate the k_{eff} of a system using two unit cell descriptions.

Consider an infinite XY-array composed of two types of fuel assemblies in a checkerboard pattern moderated by water. Each assembly consists of a 17 × 17 × 1 array of zirconium-clad, enriched UO_2 fuel pins in a square pitched array. In one array the uranium is 3.5%-enriched and in the other array the uranium is 2.9%-enriched. The UO_2 has a density of 9.21 g/cm^3. The pin diameter is 0.8 cm and is 366 cm long. The clad is 0.07 cm thick, and the pitch is 1.3 cm. Each fuel bundle is contained in a 0.65-cm-thick Boral sheath. The bundles are separated by an edge-to-edge spacing of 1.0 cm. The water and zirconium is input in the standard composition data once for every unit cell in which it appears because a material may appear in only one unit cell. Determine the k_{eff} of the infinite array. Note that periodic boundary conditions are required to obtain an infinite checkerboard array. Input data for this problem follow.

```
=CSAS6
2
S
Q
U
A
R
E
F
U
E
L
A
S
S
E
M
B
L
I
E
S
E
X
A
M
P
L
E
I
N
A
N
```

(continues on next page)


```
N
F
I
N
```

(continued from previous page)

```
V7
-238

R
E
A
D
C
O
M
P

U
O2  1
D
E
N
=9
.21 1
.0 293
. 92235 3
.5 92238 96
.5
E
N
D

Z
R   2  1
E
N
D

H2
O  3  1
E
N
D

U
O2  4
D
E
N
=9
.21 1
.0 293
. 92235 2
.9 92238 97
.1
E
N
D

Z
R   5  1
E
N
D
```

(continues on next page)

(continued from previous page)

```
H2
O  6  1
E
N
D

B4
C  7  0
.367
E
N
D

A
L   7  0
.636
E
N
D

E
N
D
C
O
M
P

R
E
A
D
C
E
L
L
D
A
T
A

L
A
T
T
I
C
E
C
E
L
L
S
Q
U
A
R
E
P
I
T
C
H
```

(continues on next page)

(continued from previous page)

```
L
A
T
T
I
C
E
C
E
L
L
S
Q
U
A
R
E
P
I
T
C
H
P
I
T
C
H
=1
.3 6
F
U
E
L
D
=0
.8 4
C
L
A
D
D
=0
.94 5
E
N
D

E
N
D
C
E
L
L
D
A
T
A
```

(continues on next page)

(continued from previous page)

```
R
E
A
D
P
A
R
A
M
F
A
R
=
Y
E
S
G
E
N
=253
E
N
D
P
A
R
A
M

R
E
A
D
G
E
O
M

U
N
I
T  1

C
O
M
='3.5 W% FUEL PIN'

C
Y
L
I
N
D
E
R 10  0
.4  2
P183
.0
```

(continues on next page)

(continued from previous page)

```
C
Y
L
I
N
D
E
R 20  0
.47 2
P183
.07

C
U
B
O
I
D   30  4
P0
.65 2
P183
.07

M
E
D
I
A 1 1 10

M
E
D
I
A 2 1 20
-10

M
E
D
I
A 3 1 30
-20
-10

B
O
U
N
D
A
R
Y 30

U
N
I
T  2
```

(continues on next page)

(continued from previous page)

```
C
O
M
='3.5 W% FUEL ASSEMBLY'

C
U
B
O
I
D  10  4
P11
.05  2
P183
.07

C
U
B
O
I
D  20  4
P11
.7   2
P183
.72

C
U
B
O
I
D  30  4
P12
.2   2
P184
.22

A
R
R
A
Y  1 10
P
L
A
C
E 9 9 1 3
*0
.0

M
E
D
I
A  7  1  20
-10
```

(continues on next page)

(continued from previous page)

```
M
E
D
I
A  3  1  20
-20
-20

B
O
U
N
D
A
R
Y  30

U
N
I
T  3

C
O
M
='2.9 W% FUEL PIN'

C
Y
L
I
N
D
E
R 10  0
.4  2
P183
.0

C
Y
L
I
N
D
E
R 20  0
.47 2
P183
.07

C
U
B
O
I
D   30  4
P0
.65 2
P183
.07
```

(continues on next page)

(continued from previous page)

```
M
E
D
I
A 4 1 10

M
E
D
I
A 5 1 20
-10

M
E
D
I
A 6 1 30
-20
-10

B
O
U
N
D
A
R
Y 30

U
N
I
T   4

C
O
M
='2.9 W% FUEL ASSEMBLY'

C
U
B
O
I
D  10  4
P11
.05  2
P183
.07

C
U
B
O
I
D  20  4
P11
.7  2
P183
.72
```

(continues on next page)

(continued from previous page)

```
C
U
B
O
I
D  30  4
P12
.2   2
P184
.22

A
R
R
A
Y  2 10
P
L
A
C
E 9 9 1 3
*0
.0

M
E
D
I
A  7  1  20
-10

M
E
D
I
A  6  1  20
-20
-20

B
O
U
N
D
A
R
Y  30

G
L
O
B
A
L
U
N
I
T 5
```

(continues on next page)

(continued from previous page)

```
C
O
M
='FUEL CASK CONTAINING 4X4 ARRAY OF ASSEMBLIES'

C
U
B
O
I
D   10  4
P24
.4  2
P184
.22

A
R
R
A
Y  3 10
P
L
A
C
E  1 1 1
-12
.2
-12
.2  0
.0

B
O
U
N
D
A
R
Y 10

E
N
D
G
E
O
M

R
E
A
D
A
R
R
A
Y
```

(continues on next page)

(continued from previous page)

```
A
R
A
=1
N
U
X
=17
N
U
Y
=17
N
U
Z
=1
F
I
L
L
F1
E
N
D
F
I
L
L

A
R
A
=2
N
U
X
=17
N
U
Y
=17
N
U
Z
=1
F
I
L
L
F3
E
N
D
F
I
L
L
```

(continues on next page)

(continued from previous page)

```
G
B
L
=3
A
R
A
=3
N
U
X
=2
N
U
Y
=2
N
U
Z
=1
F
I
L
L 2 4 4 2
E
N
D
F
I
L
L

E
N
D
A
R
R
A
Y

R
E
A
D
B
O
U
N
D
S
X
Y
F
=
P
E
R
I
O
D
I
C
```

(continues on next page)

(continued from previous page)

```
E
N
D
D
A
T
A

E
N
D
```

EXAMPLE 2. CSAS6 – Calculate the k_{eff} of a system using two unit cell descriptions and cell-weighted mixtures.

Consider a problem in which a stainless steel cylinder with an inner diameter of 56 cm and an inside height of 91 cm is filled with pellets of UO_2 in borated water. The steel is 0.125 cm thick. The spherical 2.57%-enriched UO_2 pellets have a diameter of 1.07 cm and are arranged in a triangular pitch array with a pitch of 1.13 cm. The spherical 2.96%-enriched UO_2 pellets have a diameter of 1.07 cm and are arranged in a triangular pitch array with a pitch of 1.12 cm. The cylindrical tank is filled half full of the 2.96% pellets in borated water, and the remainder is filled with the 2.57%-enriched pellets in borated water.

Mixture 100 is the cell-weighted mixture containing the 2.57%-enriched uranium pellets and mixture 200 is the cell-weighted mixture containing the 2.96%-enriched uranium pellets. Determine the k_{eff} of this system. Input data for this problem follow.

```
=CSAS6
2
.57
%
A
N
D 2
.96
%
E
N
R
U
O2
P
E
L
L
E
T
S
I
N 3500
P
P
M
B
O
R
A
T
E
D
W
A
T
E
R
```

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```
V7
-238

R
E
A
D
C
O
M
P

U
O2    1 0
.925  283 92235 2
.57 92238 97
.43
E
N
D

H2
O    2 1
.0 283
E
N
D

A
T
O
M
B
A
C
I
D 2 2
.0017
-2 3 5000 1 1001 3 8016 3 1
.0 283
E
N
D

U
O2    3 0
.925  283 92235 2
.96 92238 97
.04
E
N
D

H2
O    4 1
.0 283
E
N
D
```

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```
A
T
O
M
B
A
C
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D 4 2
.0017
-2 3 5000 1 1001 3 8016 3 1
.0 283
E
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S
S304 5 1
.0 283
E
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E
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R
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A

L
A
T
T
I
C
E
C
E
L
L
C
E
L
L
M
I
X
=100
```

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```
L
A
T
T
I
C
E
C
E
L
L
C
E
L
L
M
I
X
=200
S
P
H
T
R
I
A
N
G
P
P
I
T
C
H
=1
.13 4
F
U
E
L
D
=1
.07 3
E
N
D

E
N
D
C
E
L
L
D
A
T
A
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```
R
E
A
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P
A
R
A
M
F
L
X
=
Y
E
S
E
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D
P
A
R
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M

R
E
A
D
G
E
O
M

G
L
O
B
A
L
U
N
I
T 1

C
Y
L
I
N
D
E
R 10 38
.0 45
.5 0
.0
```

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```
C
Y
L
I
N
D
E
R 20 38
.0 91
.0 0
.0

C
Y
L
I
N
D
E
R 30 38
.125 91
.0
-0
.125

M
E
D
I
A 100 1 10

M
E
D
I
A 200 1 20
-10

M
E
D
I
A   5 1 30
-20

B
O
U
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D
A
R
Y 30

E
N
D
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E
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E
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A
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E
N
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k_{eff}.. _STARBUCS:

CHAPTER

ELEVEN

STARBUCS: A SCALE CONTROL MODULE FOR AUTOMATED CRITICALITY SAFETY ANALYSES USING BURNUP CREDIT

G. Radulescu and I. C. Gauld

STARBUCS is an analysis sequence in SCALE for automating criticality safety and burnup loading curve analyses of spent fuel systems employing burnup credit. STARBUCS requires only the fresh fuel composition, an irradiation history, and the KENO model for a spent fuel configuration to be provided in an input file. It automatically performs all necessary calculations to determine spent fuel compositions, self-shielded cross sections, and the k_{eff} of the spent fuel configuration. In addition, for burnup loading curve analyses, STARBUCS performs iterative calculations to search for initial fuel enrichments that result in an upper subcritical limit. STARBUCS allows the user to simulate axial- and horizontal-burnup gradients in a spent fuel assembly, select the specific actinides and/or fission products that are to be included in the criticality analysis, and apply isotopic correction factors to the predicted spent fuel nuclide inventory to account for calculational bias and uncertainties. A depletion analysis calculation for each of the burnup-dependent regions of a spent fuel assembly, or any other system containing spent nuclear fuel, is performed using the ORIGEN-ARP sequence of SCALE. For criticality safety calculations employing multigroup cross section data, the spent fuel compositions are used to generate resonance self-shielded cross sections for each region of the problem. The region dependent nuclide concentrations and cross sections are applied in a three-dimensional criticality safety calculation using the KENO code. Both KENO V.a and KENO-VI criticality codes are supported for single criticality safety calculations using burnup credit, but only KENO V.a can be used in criticality calculations for burnup loading curve analyses. Although STARBUCS was developed specifically to address the burnup-credit analysis needs for spent fuel transport and storage applications, it provides sufficient flexibility to allow criticality safety assessments involving many different potential configurations of UO_2 spent nuclear fuel.

11.1 Introduction

The U.S. Nuclear Regulatory Commission (NRC) issued Revision 3 of the Interim Staff Guidance 8 (ISG-8) ([Com12]) on burnup credit in September, 2012. ISG-8 provides guidance on the application of burnup-credit in criticality safety analyses for pressurized-water reactor (PWR) spent fuel in transportation and storage casks. Burnup credit is the concept of taking credit for the reduction in reactivity in spent fuel due to burnup. The reduction in reactivity that occurs with fuel burnup is due to the change in concentration (net reduction) of fissile nuclides and the production of actinide and fission-product neutron absorbers. In contrast to criticality safety analyses that employ a fresh-fuel assumption (i.e., conservatively assuming unirradiated fuel compositions), credit for burnup requires the prediction of both fissile material and absorber nuclide concentrations in spent nuclear fuel (SNF) and consideration of many burnup-related phenomena, in addition to the criticality issues.

Consideration of the depletion aspects in the criticality assessment of SNF places an increasing reliance on computational tools and methods, and significantly increases the overall complexity of the criticality safety analysis. The use of spent fuel nuclide concentrations in the criticality evaluation also necessitates consideration of many additional sources of uncertainty associated with fuel depletion. ISG-8 highlights, for example, the need for applicants employing burnup credit in criticality safety assessments to address the axial and horizontal variation of the burnup within a

spent fuel assembly, uncertainties and bias in the nuclide predictions, and the additional reactivity margin available from fission products and actinides not credited in the licensing basis.

To assist in performing and reviewing criticality safety assessments of transport and storage casks that apply burnup credit, a new control sequence called STARBUCS (**St**andardized **A**nalysis of **R**eactivity for **Bu**rnup **C**redit using **S**CALE) was developed in SCALE 5. STARBUCS automates the generation of spatially-varying nuclide compositions in a spent fuel assembly, and applies the assembly compositions in a three-dimensional (3-D) Monte Carlo analysis of the system. STARBUCS automatically prepares input files for each of the modules in the sequence, executes the modules through the SCALE driver, and performs all flow control, module interface, and data management functions. The STARBUCS sequence uses well-established code modules currently available in SCALE. STARBUCS also performs iterations over a range of initial fuel enrichments to determine the initial enrichments below which UO_2 commercial spent fuel may be loaded in a transport/storage cask for specified burnup values. With this capability, STARBUCS assists in generating burnup loading curves for criticality safety analyses of spent fuel in transport and storage casks.

The STARBUCS sequence automates the depletion calculations using the ORIGEN-ARP methodology to perform a series of cross section preparation and depletion calculations to generate a comprehensive set of spent fuel isotopic inventories for each spatially-varying burnup region of an assembly. The spent fuel nuclide concentrations are subsequently input to either CSAS5 or CSAS6 to and perform a criticality calculation of the system using the KENO V.a or KENO-VI code, respectively, to determine the neutron multiplication factor (k_{eff}) for the system. Only minimal input is required by the user to perform a typical burnup-credit analysis. The user can specify the assembly-average irradiation history, the axial density variation of the reactor moderator, the axial- and horizontal-burnup profile, and the nuclides that are to be applied in the criticality safety analysis. Nuclide correction factors may also be applied to the predicted concentrations to account for known bias and/or uncertainty in the predicted SNF compositions.

11.2 Methodology

The STARBUCS control module is a burnup-credit sequence designed to perform 3-D Monte Carlo criticality safety calculations that include the effects of spatially-varying burnup in SNF configurations. STARBUCS offers two options: either perform a single criticality safety calculation with burnup credit or perform iterative calculations for burnup loading curve analyses of commercial UO_2 spent fuels. The sequence contains a set of instructions designed to automatically process input data, execute code modules currently available in SCALE for depletion, resonance cross section, and criticality calculations. In addition, for burnup loading curve analyses, STARBUCS checks whether k_{eff} converges to a user-provided upper subcritical limit, adjusts the initial fuel enrichment using the least squares method, and repeats the sequence until either convergence is achieved or determine that no solution can be found. The overall program structures and flow for a single criticality calculation and for burnup loading curve calculations are illustrated in Fig. 11.1 and Fig. 11.2, respectively.

The sequence uses well-established code modules currently available in the SCALE code system. These modules include ARP and ORIGEN to perform the depletion analysis phase of the calculations. ORIGEN-ARP is a sequence within the SCALE system that serves as a faster alternative to the TRITON depletion sequence of SCALE to perform point-irradiation calculations with the ORIGEN code using problem-dependent cross sections. ARP uses an algorithm that enables the generation of cross section libraries for the ORIGEN code by interpolation over pregenerated cross section libraries. The ORIGEN code performs isotopic generation and depletion calculations to obtain the spent fuel nuclide compositions. For criticality safety calculations using multigroup cross section data, problem dependent cross sections are processed with the resonance self-shielding capabilities of XSProc using the region-dependent compositions from the depletion analyses. Finally, the region dependent nuclide concentrations and cross sections are applied in a 3-D criticality calculation for the system using either KENO V.a or KENO-VI to calculate the k_{eff} value.

The ORIGEN-ARP depletion analysis methodology represents a significant increase in computational speed as compared to equivalent calculations performed using the SCALE depletion analysis sequences that use two-dimensional transport methods, with virtually no sacrifice in accuracy. ARP uses an algorithm that enables the generation of cross sections for the ORIGEN code by interpolating on cross sections available in pre-generated data libraries. For uranium-based fuels the interpolation parameters available are initial fuel enrichment, burnup and, optionally, moder-

ator density. STARBUCS creates input files for ARP and ORIGEN for each burnup-dependent region of an assembly and calculates the spent fuel nuclide concentrations for the region using a user-specified assembly irradiation history, cooling time, and burnup profiles. The ORIGEN libraries must be available in advance of a STARBUCS burnup-credit calculation. These libraries may be created using TRITON. The libraries include the effects of assembly design and operating conditions on the neutron cross sections used in the burnup analysis. Several ORIGEN libraries are distributed in the SCALE code system and can be applied in a STARBUCS analysis. Alternatively, a user may create a specific ORIGEN library for other assembly types or operating conditions not available in the default libraries. The generation of ORIGEN reactor libraries is discussed in the ORIGEN Reactor Libraries chapter.

The depletion phase of the analysis is performed using ARP and ORIGEN to calculate the compositions of each discrete fuel region (axial or horizontal). After a single ORIGEN-ARP depletion calculation is completed, control is passed back to the STARBUCS module which reads the spent fuel nuclide inventories generated by ORIGEN, saves them, prepares the ARP and ORIGEN input files for the next burnup region, and executes the codes in sequence. This cycle continues until the fuel compositions for all axial and horizontal regions have been calculated and saved, completing the depletion phase of the analysis. The depletion calculations for each axial and radial zone are performed using an initial fuel basis of 1 MTHM (10:sup:*6* g heavy metal).

After all depletion calculations are completed, STARBUCS reads the spent fuel nuclide inventories for all regions and prepares input for the criticality calculation. The concentrations of all nuclides in the ORIGEN depletion analysis are converted from gram-atom units (per MTU) to units of atoms/b-cm applied in the criticality calculation. The criticality calculation is performed using the capabilities in the CSAS5 or CSAS6 control module of SCALE. Specifically, STARBUCS prepares input for the CSAS5 module when criticality calculations are to be performed using KENO V.a, and for the CSAS6 sequence when using KENO-VI. Note that only the criticality safety sequence CSAS5 of SCALE can be used for burnup loading curve calculations.

For burnup loading curve iterative calculations, STARBUCS employs the search algorithm described in CSAS5 section on *Optimum (Minimum/Maximum) Search* to determine initial fuel enrichments that satisfy a convergence criterion for the k_{eff} of the spent fuel configuration. If convergence is not achieved in a search pass, the initial fuel enrichment is automatically adjusted. This sequence repeats until either k*eff* converges to an upper subcritical limit or until the algorithm determines that a solution is not possible. The procedure is repeated for each requested burnup value. The maximum allowable iterations, upper subcritical limit, tolerance for convergence, and a range of initial fuel enrichments can be set by the user. The lower and upper enrichment bounds as well as the burnup values for spent fuel regions must be contained within the range of enrichment and burnup values used to generate the applicable ORIGEN library. The control module prepares a STARBUCS input file for each search pass requesting a single criticality calculation using the calculated spent fuel compositions. In this input file, the burnup history data block and/or the fuel mixture compositions are updated based on the outcome of the search sequence. The pre-burnup compositions for the two minor uranium isotopes, ^{234}U and ^{236}U, are updated in the STARBUCS input file for a new pass only if they were included in the initial input file prepared by the user. Their updated weight percentages are based on the assumption that the mass ratios ^{234}U/^{235}U and ^{236}U/^{235}U do not change with fuel enrichment.

11.3 Capabilities and Limitations

STARBUCS is designed to facilitate criticality safety analyses employing burnup credit by automating and linking the depletion and criticality calculations. The STARBUCS sequence has been designed to readily allow analysts and reviewers to assess the subcritical margins associated with many of the important phenomena that need to be evaluated in the context of the current regulatory guidance on burnup credit. However, STARBUCS is sufficiently general to allow virtually any configuration involving irradiated nuclear material to be analyzed. Limitations and some of the key capabilities of the STARBUCS sequence are described below.

1. STARBUCS limitations include the use of a single UO_2 fuel type and, for analyses employing multigroup cross section data, the use of geometry configurations consisting of spent fuel rod arrays. However, the type of spent fuel configurations that can be analyzed is entirely general. STARBUCS can be used to perform criticality safety assessments of individual fuel assemblies, a spent fuel cask, a spent fuel storage pool, or any nuclear system containing UO_2 irradiated nuclear fuel.

Fig. 11.1: Modules and flow of STARBUCS sequence for criticality calculations.

Fig. 11.2: Modules and flow of STARBUCS sequence for burnup loading curve calculations.

2. Only the criticality safety sequence CSAS5 of SCALE can be used for burnup loading curve calculations; therefore KENO V.a geometry description must be available in a STARBUCS input file for burnup loading curve calculations.
3. Burnup calculations can incorporate any desired operating history. The user may enter the specific power, cycle lengths, cycle down time, post-irradiation cooling time, etc. The axial-water-moderator density variation may also be specified in the depletion analysis, provided the ORIGEN cross section library contains such data.
4. The effects of assembly design, soluble boron concentrations, burnable poison exposure, reactor operating conditions, etc., are accounted for in the ORIGEN cross section libraries used in the ORIGEN depletion calculations. Libraries for several fuel assembly designs are distributed with SCALE. These libraries can also be readily created for any reactor and fuel assembly design that can be represented in the depletion analysis sequences of the SCALE system.
5. The user can select the specific actinide and/or fission product nuclides to be included in the criticality safety analysis. The user also has the option to perform a criticality calculation employing all nuclides for which cross section data exist.
6. Isotopic correction factors may be input to adjust the calculated nuclide inventories to account for known bias and/or uncertainties associated with the depletion calculations.

Minimal user input is required to perform many types of analyses. Default values are supplied for many of the input parameter keywords. The user may select from built-in burnup-dependent 18-axial-zone profiles taken from [LFKR98], or the user may input an arbitrary user-defined burnup distribution with up to 100-axial zones and up to 7-horizontal zones. The depletion analysis calculations for each zone are performed for all nuclides (the ORIGEN data libraries contain cross section and decay data for more than 1000 unique actinides, fission products, and structural activation products). The specific nuclides to be considered in the k_{eff} analysis may be input by the user. If no nuclide set is explicitly selected, then all nuclides that have cross section data in the ORIGEN library are automatically applied in the criticality analysis, resulting in a "full" burnup-credit criticality assessment. A capability to adjust the calculated isotopic inventories using correction factors that can account for biases and/or uncertainties in the calculated isotopic concentrations is also provided.

An appropriate ORIGEN cross section library for UO_2 fuel must be available for the depletion analysis using STARBUCS. The user may use the libraries distributed with SCALE (e.g., ge7×7-0, ge8×8-4, ce14×14, w15×15, w17×17_ofa) or the user may generate their own problem-specific libraries using the TRITON depletion analysis sequence available in SCALE. A complete list of ORIGEN libraries distributed with SCALE and methods for generating ORIGEN libraries are both described in the ORIGEN Reactor Libraries chapter. The range of initial fuel enrichment and requested burnup values to be used in the STARBUCS calculations must be contained within the range of the enrichments and burnups used to generate the applicable ORIGEN library.

The user is required to provide a complete KENO V.a model of the spent fuel configuration for burnup loading curve calculations and a complete KENO V.a or KENO-VI model of the spent fuel configuration for single criticality calculations using burnup credit. The initial material composition information is defined in a standard composition data block. The fuel material is automatically depleted in the sequence for each of the burnup-dependent regions or zones in the problem. The nuclide concentrations after irradiation and decay are automatically applied to the KENO criticality analysis. The mixture numbers for each of the fuel regions are identified by unique mixture numbers assigned automatically by STARBUCS based on the axial and horizontal regions in the problem (see Fig. 11.3). The user is required to specify the geometry/extent of the axial and horizontal zones in the KENO model and apply the appropriate mixture numbers for the desired configuration based on the mixture identifying scheme. STARBUCS performs no checking of the criticality model to verify that all mixtures in the problem have been used or that the order of the mixture numbers in the KENO model corresponds to the corresponding order of the input burnup profile. This provides the user a great deal of flexibility in setting up problems. However, it also requires that the user accurately prepare the input files to ensure that the spent fuel zone mixtures are assigned to the correct KENO V.a or KENO-VI geometry regions. For instance, the user could (intentionally) reverse the order of the axial-material identifiers in the KENO model to simulate inverted fuel, or zone mixtures could be omitted to simulate a problem using only a subset of the available fuel zones that were simulated in the depletion analysis.

There are several conventions that must be followed when using STARBUCS. In general, these relate to the specifica-

Fig. 11.3: Fuel and material mixture numbering convention used in STARBUCS.

Lattice element contains FUEL, GAP, CLAD, and MODERATOR

NHZ=4; NAX=25

	FUEL NHZ							Available mixture numbers		
	1	2	3	4	CLAD	MOD	GAP			
1	101	201	301	401	2	3	4	801	.	.
2	.	.	.	.	502	602	702	.	.	.
3	.	.	.	.	.	.	.	.	.	.
4	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.
.	125	225	325	425	.	.	.	.	.	.
.	126	226	326	426	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	2147
.	.	.	.	.	.	.	.	.	.	
	Available mixture numbers				.	.	.	.	.	
					.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	
100	200	300	400	500	600	700	800	.	.	

- Fuel mixture numbers
- Mixture numbers available for additional geometry materials
- Moderator mixture numbers
- Gap mixture numbers
- Clad mixture numbers

Fig. 11.4: Example of mixture numbering scheme used in STARBUCS.

tion of materials and mixture numbering of the cross section mixing table.

1. The maximum number of horizontal zones is restricted to seven if there is no gap or second moderator mixture, six if a gap or second moderator mixture is defined, and five if both a gap and a second moderator are defined. The number of axial-fuel zones is limited such that the product of horizontal zones axial zones is less than or equal to 100. These limits constrain the maximum mixture number used for burned fuel in the KENO criticality calculation to less than 1000 and assign unique mixture numbers to clad, moderator, and gap mixtures for lattice cell descriptions. The convention used to number the depleted fuel zones is to start at mixture 101 and increment by 1 for each axial-burnup region. Thus, for a case with 10 axial-burnup regions, the fuel mixtures used in the criticality analysis would range from 101 to 110. For a similar case having two horizontal zones in addition to the axial zones, the mixture numbers would also include mixtures 201 to 210.

2. Mixture numbers for the clad, gap (if applicable), and moderator may also be used directly in the KENO model. Additional unique mixture numbers are required by the code for the lattice cell descriptions for each separate fuel zone (except for mixture 0 for void). These additional mixtures are assigned automatically by the code and are shown in Fig. 11.3 for a lattice cell consisting of fuel, gap, clad, and moderator. The additional mixture numbers may also be used directly in the KENO model. Mixture number allocation is illustrated in Fig. 11.4 for an example case where the number of different horizontal zones is four and the maximum number of axial zones is limited to 25.

3. All structural materials in the problem must have mixture numbers different from the numbers automatically generated by the code (see Fig. 11.4 for an example of available mixture numbers). For the example shown in Fig. 11.4, mixtures 5–100, 126–200, 226–300, 326–400, 501, 601, 701, 426–500, and 801–2147 are not allocated by STARBUCS and may be defined by the user in the composition data block and used in the geometry model. If the constraints in paragraph 1 are followed, mixture numbers less than 100 that were not used for fuel, gap, clad, moderator and mixture numbers from 1001 to 2147 are always available for structural materials. Note that STARBUCS does not provide a warning or stop program execution if a mixture number assigned to a structural material has also been generated internally by the computer code. The mixture numbers for structural materials are not changed and are thus applied in the KENO model in a one-to-one correspondence with the standard composition mixture as done for typical CSAS calculations. Therefore, the use of a mixture number for structural materials that is identical to one of the mixture numbers automatically generated by the code results in the combination of both materials in the composition for the mixture number.

4. Not all SCALE standard composition alphanumeric names (see the Standard Composition Library chapter) are currently recognized by STARBUCS. The use of special materials (e.g., C-GRAPHITE, NIINCONEL, H-POLY), particularly as fuel materials, that have nuclide identifiers that are not readily translated to ORIGEN ZA numbers should be avoided since these materials cannot be depleted.

5. A single STARBUCS calculation is limited to a single initial fuel type (composition, enrichment, assembly design, etc.). Configurations involving multiple fuel types may be solved by running a separate STARBUCS case for each type, saving the corresponding CSAS cases generated by STARBUCS that contain the irradiated fuel nuclide compositions, and manually merging the cases in such a way that all required fuel types are represented in the final case.

11.4 Input Description

STARBUCS input is divided into different data blocks containing related types of information. The standard composition data block used to define initial (fresh) fuel composition and all other materials in the criticality analysis problem, is read and processed by the material and cross section processing module of SCALE (XSProc) and conforms to the standard input conventions (see Chapter 7 (SECTIONREFERENCE) In addition to the standard composition data, three more input data blocks are required by STARBUCS. The data blocks are entered in the form

```
R
E
A
D
X
X
X
X
i
```

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where **XXXX** is the data block keyword for the type of data being entered. The types of data blocks that are entered include general control parameter information, irradiation history and decay data or search parameter data, and the KENO V.a or KENO-VI input specifications. The valid block keywords for a single criticality safety calculation using burnup credit and for burnup loading curve calculations are listed in Table 11.1 and Table 11.2, respectively. A minimum of four characters is required for most keywords. The exception is the criticality model input data block READ KENOVA or READ KENOVI in which case the code must check additional character positions to determine the CSAS control sequence to be executed. The keywords can be up to twelve characters long, the first four of which must be input exactly as listed in the table. Entering the words **READ XXXX** followed by one or more blanks activates the data block input. All input data pertinent to block **XXXX** are then entered. Entering **END XXXX** followed by two or more blanks terminates data block **XXXX**.

Table 11.1: Valid data block keywords for a single criticality safety calculation using burnup credit

Data block type	**Block keyword**
Control parameters	CONTROL
Burnup history	HISTORY or BURNDATA
KENO V.a input	KENOVA or KENO5
KENO-VI input	KENOVI or KENO6

Table 11.2: Valid data block keywords for burnup loading curve calculations.

Data block type	**Block keyword**
Control parameters	CONTROL
Search parameters	SEARCH
KENO V.a input	KENOVA or KENO5

All input within a data block is entered using keywords and is free format. Keyword entries may be of variable or array type. Variable keyword entries include the keyword plus the "=", followed by the value. Array keywords are usually followed by a series of entries, each separated by a blank or comma, and must always be terminated with an END that does not begin in column one. In some instances a single value may be input as an array entry; however, the word END is still always required. Within a given input data block the keyword entries may be in any order.

A single data entry may be entered anywhere on a line but cannot be divided between two lines; however, array data entries may be divided over many lines. The code identifies data keywords using only the first four (maximum) characters in the keyword name. Beyond the first four characters, the user may enter any alphanumeric or special character acceptable in FORTRAN, including single blanks, before the "=" character. Floating-point data may be entered in various forms; for example, the value 12340.0 may be entered as: 12340, 12340.0, 1.234+4, 1.234E+4, 1.234E4, or 1.234E+04. Also, the value 0.012 may be entered as 12E3, 123, 1.22, etc. Numeric data must be followed immediately by one or more blanks or a comma.

11.4.1 Overview of input structure

An overview of the input to the STARBUCS sequence is given in Table 11.3. This table provides an outline of the input data block structure. The input data in positions 1 to 5 (see Table 11.3) are read and processed by the material and cross section processing module of SCALE (XSProc). These are the first data read by the code and must be in the order indicated. Data positions 6, 7 or 8, and 9 are read directly by STARBUCS and may be entered in any order.

Table 11.3: Outline of input data for the STARBUCS sequence

Data position	Type of data	Data entry	Comments
	Sequence name	=STARBUCS	Start in column one
1	TITLE	Enter a title	80 characters
2	Standard SCALE pointwise or multigroup cross section library name or the name of a user-supplied multigroup cross section library	Library name	The currently available standard SCALE cross section libraries are listed in the SCALE Cross Section Libraries chapter, table *Standard SCALE Cross-Section Libraries*. STARBUCS allows a non-standard SCALE multigroup cross section library to be used in a criticality calculation.
3	Standard Composition specification data	Enter the appropriate data	Begins this data block with READ COMP and terminate with END COMP. See Standard Composition section for details.
4	Type of calculation	LATTICECELL	Begins this data block with READ CELL and terminates with END CELL. Only regular unit cells may be used. See XSProc section for details.
5	Unit cell geometry specification[a]	Enter the appropriate data	Each dimension may be entered as a diameter. See XSProc section for LATTICECELL.
6	Control parameter data	Enter the desired data	Begins this data block with READ CONT and terminate with END CONT. See Conntrol parameter data sec
7[b]	Burnup history specification	Enter the desired data for each cycle	Begins this data block with READ HISTORY (or BURNDATA) and terminate with END HISTORY (or BURNDATA). See Burnup hist/ ory data sec.
8[b]	Search parameter data	Enter the desired data	Begins this data block with READ SEARCH and terminate with END SEARCH. See Search para/ meter data sec.
9	KENO data	En-	Begins this data block with READ KEN-

11.4.2 Sequence specification card

The STARBUCS analytical sequence is initiated with "=STARBUCS" beginning in column 1 of the input. This instructs the SCALE driver module to execute the STARBUCS sequence. The input data are then entered in free-format. The input is terminated with the word "END" starting in column 1. An "END" is a special data item, which may be used to delimit an input data block, end an array of input items, and terminate the input for the case. In the context of input data blocks, the "END" has a name or label associated with it. An "END" used to terminate an array of entries must not begin in column 1 as this instructs the SCALE driver to terminate input to the sequence.

11.4.3 Optional sequence parameters

To check the input data, run STARBUCS and specify PARM=CHECK or PARM=CHK after the analytical sequence specification as shown below.

```
=STARBUCS PARM=CHK
```

Other optional input for the PARM field to control multigroup resonance self-shielding calculations are described in the XSProc section of this manual.

11.4.4 XSProc

The XSProc is used to read and process the standard composition specification data that define the initial compositions of the fuel and all structural materials in the problem, into mixing tables and unit cell geometry information that are used by STARBUCS. All composition data required for the problem are entered as standard composition entries. A detailed description of this portion of the input can be found in the section on XSProc (Chapter 7 (SECTIONREFERENCE)). Only one UO_2 fuel type is permitted in STARBUCS. Therefore, a single fuel mixture defining the fresh fuel composition and, for criticality safety calculations employing multigroup cross sections, the geometry description of a single fuel lattice cell are required in a STARBUCS input file. Only the regular unit cells SQUAREPITCH, TRIANGPITCH, SPHSQUAREP, SPHTRIANGP, and SYMMSLACELL may be specified for the LATTICECELL entry. Outside diameters of the fuel, gap, and clad mixtures (i.e., not the radii) are required.

11.4.5 Control parameter data

The control parameter data block allows the user to specify control parameters and array data related to many of the burnup-credit analysis parameters to be used in the problem. All input is by keyword entry. All keywords are three-character identifiers that must be followed immediately by an equals sign ("="). The keywords may be in any order within a data block. Input to the parameter data block is initiated with the data block keywords **READ CONTROL** (only first four characters of block name are required). The data block is terminated by the keywords **END CONTROL**.

The types of control parameter data that may be input are summarized in Table 2.3.4. The individual keyword entries are described below.

1. ARP= NAME OF THE ORIGEN LIBRARY TO BE USED. A character string with the name of the ORIGEN library to be used in the depletion calculation. This is a required entry. The library must be defined in the SCALE text file ARPDATA.TXT that contains the cross section library names and interpolation data used by ARP. A description of an ARP input and the location of the ORIGEN cross section libraries are provided in *ARP Input Description* located in the ORIGEN ARP Module chapter. STARBUCS calculations are limited to UO_2 spent fuels.
2. NAX= NUMBER OF AXIAL ZONES. This is the number of axial-burnup subdivisions. For a user-input profile the value of NAX is determined automatically by the code, and the NAX keyword is optional, provided the AXP= array has been entered. The maximum value of NAX must be chosen such that due product of NAX

* NHZ is less than or equal to 100 (i.e., NAX:sub:*max* is 100, 50, 33, 25, 20, 16, or 14 when the number of horizontal zones is 1, 2, 3, 4, 5, 6, or 7, respectively). By default, the profile is automatically normalized to unity by the code unless NPR=no. Built-in burnup-dependent 18-axial-zone profiles may be selected with an entry of –18. These built-in profiles and the burnup range over which they are applied, are listed in Table 11.5. These profiles have been proposed elsewhere (Ref. 2) as bounding axial profiles and are included as options for convenience only. The default value of NAX is –18 (use built-in profiles).

3. NHZ= NUMBER OF HORIZONTAL ZONES. This is the number of horizontal-burnup subdivisions in the assembly. An optional entry if no horizontal profile is requested. The maximum value is seven zones. The exact limit is determined by the number of mixtures defined in the lattice cell description. If a gap and second moderator type are used the number of horizontal zones is limited to five.

4. NUC= BURNUP-CREDIT NUCLIDES used in the criticality calculation. A list of actinides and/or fission products that are to be included in the KENO criticality safety calculation. This is an array entry keyword and is delimited by the keyword END. The nuclides are entered using their standard composition alphanumeric names, as listed in the Standard Composition Library chapter of the SCALE manual. Isotopic correction factors may be entered, optionally, immediately following the nuclide name. The isotopic correction factors will be multiplied times the spent fuel nuclide concentrations to account for isotopic composition bias. The concentration of any nuclide that does not have a correction factor is not adjusted. To select all available actinide and fission product nuclides (with cross section data and atom densities greater than 1.0E29) for the criticality calculation, the user may select NUC= ALL, without an END terminator. This is the only situation where an array entry does not require an END. Note that the set of nuclides tracked by ORIGEN in any decay or irradiation calculation, documented in the ORIGEN Reaction Resource Contents chapter, is much larger than the set of nuclides with available cross sections for neutron transport calculations, documented in the SCALE Cross Section Libraries chapter. Only nuclides with available cross sections for neutron transport calculations are included in the irradiated fuel compositions for criticality calculations.

5. FLE= FUEL LIGHT ELEMENT NUCLIDES. A user-provided list of light element nuclides that are to be included in the irradiated fuel compositions for a CSAS5 or a CSAS6 calculation. This is an array entry keyword and is delimited by the keyword END. The nuclides are entered using their standard composition alphanumeric names, as listed in Standard Composition Library chapter of the SCALE manual. To select all available light element nuclides (with cross section data and atom densities greater than 1.0E29) for the criticality calculation, the user may specify FLE= ALL, without an END terminator. This is the only situation where an array entry does not require an END. The use of the keyword FLE is not required if only o-16 is to be included in the composition of irradiated uranium oxide fuel pellets. For these material mixtures, o-16 will be automatically included in irradiated fuel compositions due to its significant concentration. Isotopic correction factors are not allowed for light element nuclides. Note that the set of nuclides tracked by ORIGEN in any decay or irradiation calculation, documented in the ORIGEN Reaction Resource Contents chapter, is much larger than the set of nuclides with available cross sections for neutron transport calculations, documented in the SCALE Cross Section Libraries chapter. Only nuclides with available cross sections for neutron transport calculations are included in the irradiated fuel compositions for criticality calculations.

6. AXP= AXIAL-BURNUP PROFILE. The user-supplied axial-burnup profile of the assembly to be used in the analysis. This entry is required unless use of the built-in burnup-dependent axial profiles shown in Table 11.5 is requested (NAX= 18). If NAX is set to anything other than 18, the AXP array must contain NAX entries. Otherwise, the value of NAX is determined automatically by the code. By default (NPR=yes), the profile is automatically normalized by the code; this may be disabled by setting NPR=no. If the burnup profile is normalized, it is implicitly assumed that the height/volume of each axial region is uniform when determining the average fuel burnup (i.e., the burnup of each axial region is equally weighted). **The user is cautioned that if fuel region subdivisions of unequal volume are used, normalization should not be applied and the user must ensure a correct correspondence between the axial-profile input and the axial regions specified in the criticality calculation. AXP** is an array entry and must be delimited by an END that must not start in the first column.

7. HZP= HORIZONTAL-BURNUP PROFILE. An optional array entry used to specify a burnup gradient across assemblies. The elements of the array are the ratios of the burnups of horizontal subdivisions in the assembly to

average assembly burnup (entry for the POWER= keyword described in *Burnup history data*). If NHZ is input, the HZP array must contain NHZ entries delimited by an END that must not start in the first column. Otherwise, the value of NHZ is determined automatically by the code. The profile will be normalized if NPR=yes (default). Sample problem 5 illustrates use of this option.

8. FIX= FIXED ASSEMBLY POWER OPTION. Option to select a constant specific power level for the depletion analysis for all axial and horizontal zones of the assembly. For FIX=yes, the depletion analysis for all zones is performed using the specific power input in the power history data block for the POWER= keyword. The irradiation time is adjusted to achieve the desired burnup. The default of FIX=no applies a variable power for all zones and a constant irradiation time as defined by the BURN= keyword.

9. NPR= NORMALIZE PROFILE. Option to control whether the user input axial- and horizontal-burnup profiles will be normalized. The input profiles are automatically normalized using NPR=yes (default). If fuel region subdivisions of unequal volume are used, NPR=NO should be specified.

10. MOD= AXIAL MODERATOR DENSITY. This is an array entry keyword and is delimited by the keyword END. The array dimension is equal to the number of axial zones (NAX entry) and the array values are provided in the same order as the AXP array elements. This input array is required only if the applicable ORIGEN library contains variable moderator density cross sections.

11. BUG= DEBUG PRINT OPTION. BUG=yes will print program debugging variables and arrays in STARBUCS. The default is BUG=no.

Table 11.4: Table of control parameter data.

Keyword name	Data type	Default value	Comments
READ CONTROL		Initiate reading the control parameter block of data	
ARP=	Character	None	Name of the ORIGEN library to be used. Required. Library must be defined in SCALE text file ARPDATA.TXT.
NAX=	Integer	18	Number of axial-burnup subdivisions in fuel assembly. The value of NAX is determined automatically if an axial profile is input using AXP= entries. The maximum value of NAX is 100. Default value (18) applies a built-in 18-axial-region - burnup profile.
NHZ=	Integer	1	Number of horizontal-burn up subdivisions. Maximum value of 5–7 zones (see Sect. 2.3.4.5). No entry is required if horizontal profile is not used.
NUC=	Character and real mixed array[a]	None	List of burnup-credit nuclides, and optionally the corresponding isotopic correction factors, to be included in the criticality calculation.[b] Array entry generally delimited by END, unless ALL is selected. Nuclides are input using their standard composition alphanumeric identifiers.
FLE=	Character array[a]	o-16	List of light element nuclides to be included in the criticality calculation.[b] Array entry generally delimited by END, unless ALL is selected. Nuclides are input using their standard composition alphanumeric identifiers.
AXP=	Real array[a]	See NAX	Axial-burnup-pr ofile array. Required if NAX > 0. NAX entries that define the axial-burnup shape. The profile is automatically normalized if NPR=YES (default). Delimited by END.
HZP=	Real array[a]	None	Horizontal-burn up-profile array. Required if

Table 11.5: Built-in burnup-dependent axial profiles, NAX= 18 from [lancaster_actinide-only_1998])

Axial zone no.	Fraction of core height	Burnup < 18 GWd/MT U	18 Burnup < 30 GWd/MT U	Burnup 30 GWd/MT U
		1	2	3
1	0.0278	0.649	0.668	0.652
2	0.0833	1.044	1.034	0.967
3	0.1389	1.208	1.150	1.074
4	0.1944	1.215	1.094	1.103
5	0.2500	1.214	1.053	1.108
6	0.3056	1.208	1.048	1.106
7	0.3611	1.197	1.064	1.102
8	0.4167	1.189	1.095	1.097
9	0.4722	1.188	1.121	1.094
10	0.5278	1.192	1.135	1.094
11	0.5833	1.195	1.140	1.095
12	0.6389	1.190	1.138	1.096
13	0.6944	1.156	1.130	1.095
14	0.7500	1.022	1.106	1.086
15	0.8056	0.756	1.049	1.059
16	0.8611	0.614	0.933	0.971
17	0.9167	0.481	0.669	0.738
18	0.9722	0.284	0.373	0.462

11.4.6 Burnup history data

The burnup history data block defines the irradiation history for the assembly. These data are entered by keyword. The keywords are summarized in Table 11.6. Only the first four characters of the keywords are required (i.e., any characters after the first four characters are optional). A minimum of two entries are required for each cycle, (1) the average assembly power (POWER=) and (2) the irradiation time (BURN=). The decay time (DOWN=), if any, at the end of the cycle, and the number of cross section libraries (NLIB=) are optional. The word END is required to delimit the entries for each cycle. The entries within a given cycle may be in any order.

The burnup history data block reading is initiated with the keywords READ HISTORY (or BURNDATA) and terminated by END HISTORY (or BURNDATA).

POWER= The average specific power of the assembly for this cycle. The units of the specific power are in MW/MTU (W/g) of initial uranium. The axial and horizontal profiles are multiplied by the specific power to achieve the desired spatially-dependent burnup profiles for the assembly when FIX=NO (default). If FIX=YES, the specific power input using this keyword is assumed to be uniform over all fuel regions (axial and horizontal) and the code will adjust the irradiation time to obtain the desired burnup for each region.

BURN= THE IRRADIATION TIME FOR THIS CYCLE. The cycle irradiation time in days.

DOWN= CYCLE DOWN TIME. An optional entry to specify the down time, in days, at the end of an irradiation cycle. The down time is simulated as an irradiation time step of effectively zero power after the irradiation cycle. The down time for the last cycle is simulated as a separate ORIGEN decay case with nine equally-spaced time steps. If a negative down time is input, the time steps are spaced logarithmically.

NLIB= LIBRARIES PER CYCLE. An optional entry to request multiple cross section libraries during a depletion cycle. If requested, the code automatically subdivides the cycle in NLIB segments of uniform duration and generates a separate library for the depletion analysis for each segment using ARP. Generating multiple libraries provides a more

accurate representation of the time-dependent cross section variation during the burnup analysis. Each segment of the cycle is assumed to have the same specific power, and no down time is assumed between each segment of the cycle.

END The word END is required to terminate the input for each cycle.

Repeat the above entries for each cycle to define the complete assembly power history.

Table 11.6: Table of power history data.

Keyword name	**Data type**	**Default value**	**Comments**
READ HISTORY (or BURNDATA)[a]			Start of burnup history data block
POWER=	Real variable	None	Average assembly power for this cycle (MW/MTU)
BURN=	Real variable	None	Cycle irradiation time (days)
DOWN=	Real variable	0	End-of-cycle decay time (days). Optional. A negative down time may be used to select logarithmic decay time intervals for the last decay case.
NLIB/CYCLE=	Integer variable	1	Number of libraries to be applied in this cycle. Optional. If multiple libraries are requested for this cycle, the cycle is subdivided into equal time segments, and an updated library is generated for each segment. No down time is simulated between segments.
END			Required. Defines the end of the data for the current cycle. Repeat the above entries for each cycle in the irradiation history. An END, not to begin in column 1, must terminate each cycle definition.
END HISTORY (or BURNDATA)*a*			End block
[a] Only the first four characters are required, i.e., HIST (or BURN).			

11.4.7 Search parameter data

The search parameter data block defines input data for burnup loading curve analyses for commercial UO_2 spent fuels. Burnup history input data are not allowed in an input file that supplies search parameters. A burnup history data block is generated in STARBUCS for subsequent iterative calculations using the initial user-supplied search parameter data. STARBUCS sample problem *starbucs1.input* contains a search data block to request burnup loading curve analyses for spent fuel at various burnups. The search data block reading is initiated with the keywords READ SEARCH and terminated by END SEARCH. The keywords are summarized in Table 11.7. These keywords may be in any order.

USL= THE UPPER SUBCRITICAL LIMIT FOR BURNUP LOADING.

EPS= TOLERANCE ON CONVERGENCE. The convergence criterion used in the search for initial fuel enrichment so that user-specified k_{eff} value is within USL $\pm$ EPS. The tolerance value must be greater that the standard deviation of the calculated k_{eff} for the solution to converge.

ITMAX= MAXIMUM ITERATIONS ALLOWED FOR EACH ENRICHMENT SEARCH. The search for initial fuel enrichment stops when the number of iterations exceeds this parameter and a warning message is provided to the user.

ECL= LOWER ENRICHMENT CONSTRAINT. The unit for this parameter is wt% ^{235}U. The lower enrichment constraint must be within the enrichment interval used in the ORIGEN library specified in READ CONTROL data block.

ECH= UPPER ENRICHMENT CONSTRAINT. The unit for this parameter is wt% ^{235}U. The upper enrichment constraint must be within the enrichment interval used in the ORIGEN library specified in READ CONTROL data block.

BU= ARRAY OF REQUESTED BURNUP VALUES (GWd/MTU). The word END is required to terminate this array. The user inputs a series of discharge burnup values for which the initial fuel enrichments that result in a desired k_{eff} value (USL $\pm$ EPS) are to be determined.

AVGBU= AVERAGE BURNUP PER CYCLE (GWd/MTU). An optional entry used to determine the number of irradiation cycles as the ratio of a burnup value in the BU array to AVGBU.

POWER= The average specific power of the assembly. The units of the specific power are in MW/MTU (W/g) of initial uranium. This entry has the same function as the entry for POWER= keyword in the HISTORY data block (see *Burnup history data*). It is also used to determine cycle irradiation time as the ratio of a burnup value in the BU array to average assembly power.

FDT= FRACTIONAL DOWNTIME. An optional entry used to determine down time between irradiation cycles (the entry for DOWN= keyword in the HISTORY data block) if fuel irradiation requires two or more cycles. For example, for a cycle with 365 days of irradiation followed by a 30-day downtime, FDT = 30 / 395 = 0.07595. STARBUCS uses the user-provided FDT to compute cycle downtime as the irradiation time per cycle multiplied by FDT and divided by (1-FDT).

DEC= DECAY TIME AFTER IRRADIATION. An optional entry to specify the decay time, in days, after fuel discharge. A negative value may be used to select logarithmic decay time intervals.

NLIB= NUMBER OF LIBRARIES PER CYCLE. An optional entry to request multiple cross section libraries during a depletion cycle. Generating multiple libraries provides a more accurate representation of the time-dependent cross section variation during the burnup analysis. Each segment of the cycle is assumed to have the same specific power.

FFE= FRESH FUEL ENRICHMENT. The purpose of this option is to help in reducing the total number of iterations needed to achieve convergence. There are two options implemented in STARBUCS for the fresh fuel enrichment value to be used in the first inner iterations over fuel enrichment, FFE=SEARCH (default) and FFE=INPUT. With the default option (FFE=SEARCH), the lower enrichment bound and the starting fresh fuel enrichment at the beginning of a search are adjusted based on the results of the previous outer iteration over burnup. The procedure includes the following steps. First, the user requested burnup values are sorted in ascending order so that STARBUCS outer iterations over burnup proceed from the lowest to the highest burnup value. Then, the initial fresh fuel for the lowest burnup is changed to the mid-value of the enrichment interval, (ECL+ECU)/2, and the search for the fresh fuel enrichment corresponding to the lowest burnup is initiated and completed. Suppose that a solution for this burnup step exists. This solution becomes the lower enrichment constraint (ECL) in the search passes for the next burnup value and the initial fresh fuel enrichment is chosen as the middle point of the enrichment interval. The procedure is applied for the entire set of the requested burnups. The average number of iterations for each burnup step with this option is approximately 4. The alternate option (FFE=INPUT) starts a search for fuel enrichment with the user supplied fresh fuel enrichment.

Table 11.7: Table of search data.

Keyword Name	Data type	Default value	Comments
READ SEARCH[a]			Initiate reading the search block of data.
USL=	Real	1.0	Upper subcritical limit.
EPS=	Real	0.005	Tolerance on convergence.
ITMAX=	Integer	10	Iteration limit.
ECL=	Real	1.5	Lower initial fuel enrichment constraint (U-235 wt%).
ECH=	Real	5.0	Upper initial fuel enrichment constraint (U-235 wt%).
BU	Real[b]	None	Array entry of requested burnup values (GWd/MTU).[c]
AVGBU=	Real	20.0	Average burnup per cycle.
POWER=	Real	25.0	Average specific power (W/g).
FDT=	Real	0.2	Fractional downtime.
DEC=	Real	1825.0	Decay time (days).
NLIB=	Integer	2	Libraries per cycle.
FFE=	Character	SEARCH	Fresh fuel option. FFE=INPUT starts the outer iterations over the burnup values with user supplied fresh fuel composition. FFE=SEARCH helps in reducing the number of search passes (approximately 4 in average).
END SEARCH		End of the search data	
[a] Only the first four characters are required. [b] Terminate array data entries with end. Do not place this end in column 1. [c] There are no restraints on the maximum number of the burnup values requested in burnup loading curve calculations. A user may consider computer time and resources in assessing the maximum number of burnup values in this array.			

11.4.8 KENO input data

The KENO input for the problem is specified in the KENO data block. Input to the data block is initiated with the data block keywords **READ KENO or READ KENOVA** and is terminated by the keywords **END KENO** or **END KENOVA** for criticality calculations using **KENO V.a**. Input to the data block is initiated with the data block keywords **READ KENOVI or READ KENO6** and is terminated by the keywords **END KENOVI** or **END KENO6** for criticality calculations using **KENO VI**. STARBUCS performs no error checking of the KENO input. The data within the data block delimiters is copied, without change, to the CSAS input file and executed. The user is therefore advised to ensure that the KENO input is free of errors by first running the case within CSAS5 or CSAS6 before applying the input in STARBUCS.

The input requirements for KENO V.a and KENO-VI are not described in this section, but are described in detail in the KENO chapter of this manual. This section describes only the input requirements as related to the execution of KENO within STARBUCS and the conventions used for module compatibility.

The mixture numbers for each of the non-fuel materials applied to the material regions of the KENO model are defined as the mixture numbers (MX) specified in the standard composition input. STARBUCS automatically defines the *MIXTURE ID* for each of the fuel regions according to the axial and/or horizontal zones defined by the NAX and NHZ entries in the burnup-profile arrays. The first axial-zone mixture is assigned MX=101, and is incremented by one for each additional axial zone. Therefore, in a problem that defines 18 axial zones, spent fuel mixtures will be generated with identifiers that range from 101 to 118. The correspondence of these mixtures to the assembly locations is determined by the ordering of the AXP= input array that defines the axial-burnup profile for the assembly. If the AXP= array orders the burnup profile from the bottom of the assembly to the top of the assembly, the resulting MX=101 will correspond to the bottom axial-zone segment, and MX=118 would correspond to the top axial zone. If multiple horizontal zones are defined, then the numbering sequence of the second horizontal zone will start at MX=201 and, in the example given here, would range up to MX=218. Refer to *Capabilities and Limitations* for limitations in the mixture-numbering scheme. The mixture-numbering scheme is illustrated in Fig. 11.3.

11.5 Sample problems

A series of example problems are presented to illustrate the application of STARBUCS to burnup-credit criticality safety and burnup loading curve analyses. Sample problem 1 is a simple pin-cell problem for burnup loading curve iterative calculations. The fuel pin contains a single axial-burnup zone (i.e., uniform-axial burnup). It is useful to illustrate the main features of the system and demonstrate functionality of the system modules within SCALE. Problem 2 illustrates the same problem with 18-axial burnup-dependent zones. Problem 3 extends the pin-cell model to an array of spent fuel assemblies residing in a water-filled pool. The models apply 18-axial-burnup-dependent zones. Problem 4 is a generic cask model, and this problem exercises more of the burnup credit options available in STARBUCS. Problem 5 illustrates the use of the horizontal-burnup option for a simple 4×4 array of spent fuel assemblies residing in water. Sample problem 6 uses KENO-VI to model a hexagonal VVER-440 fuel assembly.

11.5.1 Sample problem 1

Sample problem 1, listed in Listing 11.1, defines a simple infinite UO_2 pin-cell model with uniform-axial burnup for burnup loading curve calculations. The initial fuel enrichment is 2.0 wt %. The control parameter data block specifies that the standard Westinghouse (W) 17×17 ORIGEN library is to be used for the depletion analysis. The burnup-credit criticality calculation uses a subset of the major actinides as defined in the NUC= array. The sample problem contains a "*read search*" data block, which provides an upper limit for subcriticality, *usl*, a tolerance value for the search algorithm, *eps*, the lower and upper enrichment bounds, *ecl* and e*ch*, respectively, the maximum number of iterations for each burnup value requested, *imaxl*, average specific power in W/g, *power*, decay time after irradiation in days, *dec*, number of libraries per cycle, *nlib*, average burnup per cycle in GWd/MTU, *avgbu*, fractional downtime, *fdt*, and a set of burnup values, *bu* array.

11.5.2 Sample problem 2

Sample problem 2, listed in Listing 11.2, illustrates a simple pin-cell model using 18-axial-burnup-dependent zones. In this example, the built-in axial profiles for three burnup ranges are applied using the NAX= 18 option (see profiles in Table 11.5). STARBUCS determines the average assembly burnup from the power history data input, and automatically selects the appropriate profile based on the discharge assembly burnup. The axial-profile data were developed for a predefined axial-zoning structure (i.e., fraction of the assembly height). It is important that the KENO V.a geometry model therefore also reflect this axial-zone structure. That is, the height of each axial zone in the criticality model must conform to the axial zones for the profile applied in the analysis. In this example, the total pin height is 365.7 cm (144 in.), which is subdivided into 18 equal-height segments of 20.32 cm each.

The burnup-dependent cross sections generated for the criticality analysis have material identifiers ranging from 101 (bottom) to 118 (top). There is no constraint on how the fuel materials can be applied in the KENO V.a model. For example, the order of the material numbers could easily be reversed, which would effectively invert the profile and could be used to simulate an assembly loaded upside down. It is also not necessary to use all of the materials in the problem. For instance, all fuel regions in the KENO V.a model could be assigned the same fuel mixture number to represent a flat axial profile having a burnup value equal to that of the particular mixture used. The average assembly burnup would also be equal to that of the particular mixture used, and not that defined by the power history data block.

Listing 11.1: STARBUCS input listing for sample problem 1

```
=
s
t
a
r
b
u
c
s

P
W
R 17
x17
F
u
e
l
A
s
s
e
m
b
l
y
-
u
n
i
f
o
r
m
a
x
i
a
b
u
r
n
```

(continues on next page)

(continued from previous page)

```
v7
-238
  read
 comp

'
U
O2
F
u
e
l 2
.0
w
t
%
u
-235

u
o2    1
d
e
n
=10
.96 0
.95 293
.0 92235 2
.0 92238 98
.0 end

'
Z
i
r
c
a
l
l
o
y

z
i
r
c4  2  1  end

'
W
a
t
e
r

h2
o    3  1  end
```

(continues on next page)

(continued from previous page)

```
'
G
a
p

n 4
d
e
n
=0
.00125 1 end
  end
 comp
  read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
q
u
a
r
e
p
i
t
c
h
p
i
t
c
h
=1
.259 3
f
u
e
l
d
=0
.805 1
c
l
a
d
d
=0
.95 2
g
a
p
d
```

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(continued from previous page)

```
  end
 celldata

'
E
n
t
e
r
b
u
r
n
u
p
c
r
e
d
i
t
c
o
n
t
r
o
l
p
a
r
a
m
e
t
e
r
s
  read
 control

a
r
p
=
w17
x17

a
x
p
= 1 end

n
u
c
=
u
-234
u
-235
u
-236
u
```

(continues on next page)

(continued from previous page)

```
p
u
-241
p
u
-242
a
m
-241
a
m
-242
m
a
m
-243
n
p
-237 end

f
l
e
=
a
l
l
  end
 control
  read
 search

u
s
l
=0
.96

e
p
s
=0
.002

e
c
l
=1
.51

e
c
h
=4
.99
```

(continues on next page)

```
i
t
m
a
x
=10
```

(continued from previous page)

```
p
o
w
e
r
=60
.0

d
e
c
=1826
.25

n
l
i
b
=2

a
v
g
b
u
=20

f
d
t
=0
.2

f
f
e
=
i
n
p
u
t

b
u
= 10 50 70  end
  end
 search
  read
 kenova

'
i
n
f
i
n
i
t
e
p
i
n
```

(continues on next page)

(continued from previous page)

```
'

'
*
*
*
```

(continued from previous page)

```
'
* 2
=
Z
i
r
c
a
l
o
y

'
* 3
=
W
a
t
e
r

'
* 4
=
G
a
p

'
*
*
*
```

(continued from previous page)

```
  read
 param
 tme
=
1
0
0
0
0
 gen
=
5
1
0
 nsk
=
1
0
 npg
=
1
0
0
0
 end
 param
  read
 geom

'
F
u
e
l
P
i
n

g
l
o
b
a
l
u
n
i
t 1

c
y
l
i
n
d
e
r   101  1   0
.4025  50
.0
=50
.0
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   4    1   0
.4110  50
.0
-50
.0

c
y
l
i
n
d
e
r   2    1   0
.4750  50
.0
-50
.0

c
u
b
o
i
d     3    1 4
p0
.6295  50
.0
-50
.0

'
  end
 geom
  read
 bounds

 all
=reflect

 end
 bounds
  end
 data
  end
 kenova
  end
```

Listing 11.2: STARBUCS input listing for sample problem 2

```
=starbucs

P
W
R 17
x17
F
u
e
l
A
s
s
e
m
b
l
y
- 18
-
z
o
n
e
a
x
i
a
l
b
u
r
n
u
p
p
r
o
f
i
l
e

v7
-238
read
 comp
' UO2 Fuel 2.0 wt% u-235

u
o2    1
d
e
n
=10
.96 0
.95 293
.0 92235 2
.0 92238 98
.0 end
```

(continues on next page)

(continued from previous page)

```
'Zircalloy

z
i
r
c4  2  1  end
'Water

h2
o    3  1  end
'Gap

n 4
d
e
n
=0
.00125 1 end
end
 comp
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
q
u
a
r
e
p
i
t
c
h
p
i
t
c
h
=1
.259 3
f
u
e
l
d
=0
.805 1
c
l
a
d
d
```

(continues on next page)

(continued from previous page)

```
end
 celldata
' Enter burnup credit control parameters
read
 control

a
r
p
=
w17
x17
n
a
x
=
-18

n
u
c
=
u
-234
u
-235
u
-236
u
-238
p
u
-238
p
u
-240

p
u
-241
p
u
-242
a
m
-241
a
m
-242
m
a
m
-243
n
p
-237 end
```

(continues on next page)

```
f
l
e
=
o
-16
h
```

(continued from previous page)

```
end
 control
read
 hist

p
o
w
e
r
=35
.001
b
u
r
n
=100
n
l
i
b
=1 end

p
o
w
e
r
=28
.5
b
u
r
n
=230
d
o
w
n
=100
n
l
i
b
=2 end

p
o
w
e
r
=24
.001
b
u
r
n
```

(continues on next page)

```
=300
n
l
i
b
=2
d
```

(continued from previous page)

```
end
 hist
read
 kenova
'*************************************
'* materials
'* 101-118 = uo2, 18-axial zone model
'* 2 = Zircaloy
'* 3 = Water
'* 4 = Gap
'*************************************
read
 param

 tme
=
1
0
0
0
0
 gen
=
5
1
0
 nsk
=
1
0
 npg
=
1
0
0
0
 end
 param
read
 geom
'           Fuel Pin

g
l
o
b
a
l
u
n
i
t 1

c
y
l
i
n
d
e
r 101 1 0
.4025
-162
.53
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   102  1  0
.4025
-142
.22
-182
.85

c
y
l
i
n
d
e
r   103  1  0
.4025
-121
.90
-182
.85

c
y
l
i
n
d
e
r   104  1  0
.4025
-101
.58
-182
.85

c
y
l
i
n
d
e
r   105  1  0
.4025
-81
.27
-182
.85
```

(continues on next page)

```
c
y
l
i
n
d
e
```

(continued from previous page)

```
c
y
l
i
n
d
e
r   107  1  0
.4025
-40
.63
-182
.85

c
y
l
i
n
d
e
r   108  1  0
.4025
-20
.32
-182
.85

c
y
l
i
n
d
e
r   109  1  0
.4025    0
.00
-182
.85

c
y
l
i
n
d
e
r   110  1  0
.4025   20
.32
-182
.85

c
y
l
i
n
d
e
r   111  1  0
.4025   40
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   112  1  0
.4025   60
.95
-182
.85

c
y
l
i
n
d
e
r   113  1  0
.4025   81
.27
-182
.85

c
y
l
i
n
d
e
r   114  1  0
.4025  101
.58
-182
.85

c
y
l
i
n
d
e
r   115  1  0
.4025  121
.90
-182
.85

c
y
l
i
n
d
e
r   116  1  0
.4025  142
.22
-182
.85
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   117  1  0
.4025  162
.53
-182
.85

c
y
l
i
n
d
e
r   118  1  0
.4025  182
.85
-182
.85

c
y
l
i
n
d
e
r   4    1  0
.4110  182
.85
-182
.85

c
y
l
i
n
d
e
r   2    1  0
.4750  182
.85
-182
.85

c
u
b
o
i
d     3    1 4
p0
.6295 182
.85
-182
.85
```

(continues on next page)

(continued from previous page)

```
'
end
 geom
read
 bounds

 all
=reflect

 end
 bounds
end
 data
end
 kenova
end
```

11.5.3 Sample problem 3

Sample problem 3, listed in Listing 11.3, performs a burnup-credit criticality safety calculation using the SCALE 238-group ENDF/B-VII cross section library (V7-238) for an array of Combustion Engineering (CE) 14 × 14 spent fuel assemblies in water. A subset of burnup-credit actinides and fission products are included in the criticality calculation. A user-supplied 18-axial-region-burnup profile of the assemblies is input. This profile was obtained from the axial-burnup-profile database [Cac00] for Maine Yankee assembly N863. Note that the axial profile will be normalized automatically by the code using NPR=yes (default). The normalization is performed such that the average value of the profile values is unity (i.e., the sum of the profile values is equal to the number of axial zones). The 3.3 wt % enriched UO_2 fuel is assumed to achieve a discharge burnup of 37,626 MWd/MTU in three cycles of approximately 12.5 GWd/MTU per cycle and a downtime per cycle of 80 days, followed by a cooling time of 5 years after discharge (1826 days). An average assembly power level of 32 MW/MTU is used for the depletion calculation. Two libraries per cycle are requested during the depletion. Note that by increasing the number of libraries generated per cycle, the cross sections used in the burnup analysis are updated more frequently to reflect the changes that occur with burnup. The nominal CE 14 × 14 assembly design specifications were obtained from [DH96]. The assembly pitch in the criticality calculations is 22.78 cm. A cross section view of the assembly geometry, a 2 × 8 array of water reflected assemblies, is illustrated in Fig. 11.5.

Listing 11.3: STARBUCS input listing for sample problem

```
=
s
t
a
r
b
u
c
s

C
E 14
x14
a
s
s
e
m
b
```

(continues on next page)

```
y 2
x 8
a
```

(continued from previous page)

```
V7
-238
read
 comp
' UO2 Fuel 3.3 wt% u235

u
o2  1
d
e
n
=10
.045 1 273 92234 0
.0294 92235 3
.3 92236 0
.0152 92238 96
.6554 end
'Zircalloy

z
i
r
c4 2  1  end
'Water

h2
o    3  1  end
end
 comp
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
q
u
a
r
e
p
i
t
c
h
p
i
t
c
h
=1
.473 3
f
u
```

(continues on next page)

(continued from previous page)

```
c
l
a
d
d
=1
.118 2
g
a
p
d
=0
.985 0  end
end
 celldata
read
 control

a
r
p
=
c
e14
x14
n
a
x
=18

a
x
p
=
  0
.67053 0
.93322 1
.02433 1
.05329 1
.06026 1
.06185
  1
.06215 1
.06249 1
.06312 1
.06408 1
.06541 1
.06702
  1
.06836 1
.06760 1
.05918 1
.02515 0
.92262 0
.66935 end
```

(continues on next page)

```
n
u
c
=
```

(continued from previous page)

```
u
-234
u
-235
u
-236
u
-238
p
u
-238
p
u
-239
p
u
-240

p
u
-241
p
u
-242
a
m
-241
n
p
-237

m
o
-95
t
c
-99
r
u
-101
r
h
-103
a
g
-109
c
s
-133
n
d
-143

n
d
-145
s
m
-147
s
m
-149
s
```

(continues on next page)

(continued from previous page)

```
e
u
-153
g
d
-155 end
end
 control
read
 hist

p
o
w
e
r
=32
.00
b
u
r
n
=391
.937
n
l
i
b
=2
d
o
w
n
=80  end

p
o
w
e
r
=32
.00
b
u
r
n
=391
.937
n
l
i
b
=2
d
o
w
n
=80  end
```

(continues on next page)

(continued from previous page)

```
p
o
w
e
r
=32
.00
b
u
r
n
=391
.937
n
l
i
b
=2
d
o
w
n
=1826 end
end
 hist
read
 keno
'
'****************************************
'* materials
'* 101 = uo2, lower axial region (0.67053)
'* 118 = uo2, upper axial region (0.66935)
'* 2 = Zircaloy
'* 3 = Water
'****************************************
read
 param

t
m
e
=10000
g
e
n
=510
n
s
k
=10
n
p
g
=1000
end
 param
```

(continues on next page)

(continued from previous page)

```
read
 geom
'  Fuel Pin

u
n
i
t           1

c
y
l
i
n
d
e
r   101  1  0
.484
-162
.53
-182
.85

c
y
l
i
n
d
e
r   102  1  0
.484
-142
.22
-182
.85

c
y
l
i
n
d
e
r   103  1  0
.484
-121
.90
-182
.85

c
y
l
i
n
d
```

(continues on next page)

```
e
r   104  1  0
.484
-101
.58
-182
.85
```

(continued from previous page)

```
c
y
l
i
n
d
e
r   105  1  0
.484
-81
.27
-182
.85

c
y
l
i
n
d
e
r   106  1  0
.484
-60
.95
-182
.85

c
y
l
i
n
d
e
r   107  1  0
.484
-40
.63
-182
.85

c
y
l
i
n
d
e
r   108  1  0
.484
-20
.32
-182
.85
```

(continues on next page)

```
c
y
l
i
n
d
e
```

(continued from previous page)

```
c
y
l
i
n
d
e
r   110  1  0
.484   20
.32
-182
.85

c
y
l
i
n
d
e
r   111  1  0
.484   40
.63
-182
.85

c
y
l
i
n
d
e
r   112  1  0
.484   60
.95
-182
.85

c
y
l
i
n
d
e
r   113  1  0
.484   81
.27
-182
.85

c
y
l
i
n
d
e
r   114  1  0
.484  101
.58
-182
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   115  1  0
.484  121
.90
-182
.85

c
y
l
i
n
d
e
r   116  1  0
.484  142
.22
-182
.85

c
y
l
i
n
d
e
r   117  1  0
.484  162
.53
-182
.85

c
y
l
i
n
d
e
r   118  1  0
.484  182
.85
-182
.85

c
y
l
i
n
d
e
r   0  1  0
.4925 182
.85
-182
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   2    1  0
.559  182
.85
-182
.85

c
u
b
o
i
d     3    1 4
p0
.7365 182
.85
-182
.85
'
'  2 x 2 Array of Fuel Pins

u
n
i
t           2

a
r
r
a
y 1 3
*0
'
'  Large Water Hole

u
n
i
t           3

c
y
l
i
n
d
e
r   3    1  1
.3140  182
.85
-182
.85
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   2    1  1
.4160  182
.85
-182
.85

c
u
b
o
i
d     3    1 4
p1
.473  182
.85
-182
.85
'
'  Assembly Unit

u
n
i
t           4

a
r
r
a
y      2
-10
.311
-10
.3124
-182
.85

c
u
b
o
i
d     3    1 4
p11
.390  182
.85
-182
.85
'
```

(continues on next page)

(continued from previous page)

```
'  Assembly Array (2x8)

g
l
o
b
a
l

u
n
i
t            5

a
r
r
a
y       3   3
*0

r
e
f
l
e
c
t
o
r   3   1  6
r30
.0   1
end
 geom
read
 array

a
r
a
=1
n
u
x
=2
n
u
y
=2
n
u
z
=1
f
i
l
l
```

(continues on next page)

(continued from previous page)

```
  1 1
  1 1  end
 fill

a
r
a
=2
n
u
x
=7
n
u
y
=7
n
u
z
=1
f
i
l
l
  2 2 2 2 2 2 2
  2 3 2 2 2 3 2
  2 2 2 2 2 2 2
  2 2 2 3 2 2 2
  2 2 2 2 2 2 2
  2 3 2 2 2 3 2
  2 2 2 2 2 2 2  end
 fill

a
r
a
=3
n
u
x
=2
n
u
y
=8
n
u
z
=1
f
i
l
l
  16
r4  end
 fill
end
 array
```

(continues on next page)

(continued from previous page)

```
read
 bounds

 all
=void

 end
 bounds
end
 data
end
 keno
end
```

11.5.4 Sample problem 4

Sample problem 4, listed in Listing 11.4, illustrates the application of STARBUCS for a criticality safety analysis of a burnup-credit cask. The cask geometry in this example is based on a 32-assembly generic burnup-credit cask model and is illustrated in Fig. 11.6.

The assemblies are assumed to be W 17 × 17 OFA assemblies with an initial enrichment of 4.98 wt %. The standard composition description for this problem includes the fuel assembly and all cask structural material definitions. The analysis applies built-in 18-axial-zone profiles, and actinide-only burnup credit (i.e., only a subset of actinides and no fission products). The assembly is irradiated to an average burnup of about 50 GWd/MTU. The axial-burnup profile is automatically selected by the code based on the average assembly burnup. Isotopic correction factors are applied to the calculated actinide inventories. The correction factors were obtained from Ref. 4. An axial-moderator density is also applied. Note that actual entries in the MOD= array are not realistic for a PWR and are only intended to illustrate the use of this feature. Since the ORIGEN library applied in this calculation does not have variable moderator density, the values in the MOD= array have no effect on the calculation. The criticality evaluation of the cask is performed following a cooling time of 1826 days (5 years).

Listing 11.4: STARBUCS input listing for sample problem 4

```
=starbucs

P
W
R 18
-
a
x
i
a
l
z
o
n
e
W17
x17
a
s
s
e
m
b
l
y
'
G
B
C
```

(continues on next page)

Fig. 11.5: Plot of the CE 14 × 14 assembly array geometry in sample problem 3.

Fig. 11.6: Cutaway view of the generic 32-assembly burnup-credit cask showing the cask bottom half with a quarter of the model removed.

(continued from previous page)

```
v7
-238
read
 comp
' UO2 Fuel Rod 4.98 wt % u235

u
o2    1
d
e
n
=10
.96 0
.95 293
.0 92235 4
.98 92238 95
.02 end
'Zircalloy

z
i
r
c2  2  1  end
'Water

h2
o    3  1  end
'Stainless Steel

s
s304  4  1  end
' BORAL Center - B-10 loading of 0.0225 g/cm3

b
-10   5  0  6
.5795
E
-03   293
.0  end

b
-11   5  0  2
.7260
E
-02   293
.0  end

c      5  0  8
.4547
E
-03   293
.0  end

a
l     5  0  4
.1795
E
-02   293
.0  end
```

(continues on next page)

(continued from previous page)

```
'Stainless Steel

s
s304  6  1  end
' aluminum

a
l     7  0  0
.0602       293
.0  end
end
 comp
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
q
u
a
r
e
p
i
t
c
h
p
i
t
c
h
=1
.2598 3
f
u
e
l
d
=0
.7844 1
c
l
a
d
d
=0
.9144 2
g
a
p
d
=0
.8001 0 end
```

(continues on next page)

(continued from previous page)

```
end
 celldata
read
 control

a
r
p
=
w17
x17
_
o
f
a
n
a
x
=
-18

n
u
c
=
u
-234 0
.635

u
-235 1
.085

u
-236 0
.910

u
-238 0
.992

p
u
-238 0
.856

p
u
-239 1
.076

p
u
-240 0
.945

p
u
-241 1
.087
```

(continues on next page)

(continued from previous page)

```
p
u
-242 0
.848

a
m
-241 0
.609

a
m
-243 0
.804

n
p
-237 0
.697 end

m
o
d
= 0
.720 0
.709 0
.699 0
.688 0
.678 0
.667 0
.657
     0
.646 0
.635 0
.625 0
.614 0
.604 0
.593 0
.583
     0
.572 0
.562 0
.551 0
.540 end
end
 control
read
 hist

p
o
w
e
r
=32
.89
b
u
r
n
=100 end
```

(continues on next page)

(continued from previous page)

```
p
o
w
e
r
=32
.89
b
u
r
n
=200 end

p
o
w
e
r
=32
.89
b
u
r
n
=900
n
l
i
b
=3 end

p
o
w
e
r
=32
.89
b
u
r
n
=320
d
o
w
n
=
-1826 end
end
 hist

read
 kenova
'*************************************
'* Assembly Type: Westinghouse 17x17 OFA/V5
```

(continues on next page)

(continued from previous page)

```
'* Materials
'* 101 - 118 = uo2, axial regions 1 through 18
'* 2 = Zircaloy
'* 3 = Water
'* 4 = Stainless Steel
'* 5 = Boral
'* 6 = Stainless Steel
'* 7 = Al

'*************************************
read
 param
 tme
=
1
0
0
0
0
 gen
=
5
1
0
 nsk
=
1
0
 npg
=
1
0
0
0
 end
 param

read
 geom

u
n
i
t 1

c
o
m
='Fuel Pin'

c
y
l
i
n
d
e
r   101  1  0
.3922
-162
.55
-182
.85
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   102  1  0
.3922
-142
.22
-182
.85

c
y
l
i
n
d
e
r   103  1  0
.3922
-121
.90
-182
.85

c
y
l
i
n
d
e
r   104  1  0
.3922
-101
.58
-182
.85

c
y
l
i
n
d
e
r   105  1  0
.3922
-81
.27
-182
.85
```

(continues on next page)

```
c
y
l
i
n
d
e
```

(continued from previous page)

```
c
y
l
i
n
d
e
r   107  1  0
.3922
-40
.63
-182
.85

c
y
l
i
n
d
e
r   108  1  0
.3922
-20
.32
-182
.85

c
y
l
i
n
d
e
r   109  1  0
.3922    0
.00
-182
.85

c
y
l
i
n
d
e
r   110  1  0
.3922   20
.32
-182
.85

c
y
l
i
n
d
e
r   111  1  0
.3922   40
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   112  1  0
.3922   60
.95
-182
.85

c
y
l
i
n
d
e
r   113  1  0
.3922   81
.27
-182
.85

c
y
l
i
n
d
e
r   114  1  0
.3922  101
.58
-182
.85

c
y
l
i
n
d
e
r   115  1  0
.3922  121
.90
-182
.85

c
y
l
i
n
d
e
r   116  1  0
.3922  142
.22
-182
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   117  1  0
.3922  162
.53
-182
.85

c
y
l
i
n
d
e
r   118  1  0
.3922  182
.85
-182
.85

c
y
l
i
n
d
e
r   0    1  0
.40005  182
.85
-182
.85

c
y
l
i
n
d
e
r   2    1  0
.4572  182
.85
-182
.85

c
u
b
o
i
d     3    1  2
p0
.6299  2
p0
.6299  182
.88
```

(continues on next page)

(continued from previous page)

```
u
n
i
t 2

c
o
m
='Guide Thimble/Instrument Tube'

c
y
l
i
n
d
e
r 3 1 0
.56135  365
.76  0

c
y
l
i
n
d
e
r 2 1 0
.602    365
.76  0

c
u
b
o
i
d   3 1  0
.6299
-0
.6299  0
.6299
-0
.6299  365
.76  0


u
n
i
t 4

c
o
m
='Top Half Horizontal Boral Panel'
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d          7  1  9
.5250
-9
.5250     0
.02540   0
.0       365
.76   0
.

c
u
b
o
i
d          5  1  9
.5250
-9
.5250     0
.12827   0
.0       365
.76   0
.

c
u
b
o
i
d          3  1  11
.75
-11
.75       0
.12827   0         365
.76   0


u
n
i
t 5

c
o
m
='Right-Hand Side Half Vertical Boral Panel'

c
u
b
o
i
d          7  1  0
.02540   0
.0       9
.5250
-9
.5250     365
.76   0
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d          5  1  0
.128270  0
.0       9
.5250
-9
.5250     365
.76   0
.

c
u
b
o
i
d          3  1  0
.12827    0       11
.75
-11
.75       365
.76   0


u
n
i
t 6

c
o
m
='Bottom Half Horizontal Boral Panel'

c
u
b
o
i
d          7  1  9
.5250
-9
.5250     0
.0
-0
.0254      365
.76   0
.

c
u
b
o
i
d          5  1  9
.5250
-9
.5250     0
.0
-0
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d          3  1  11
.75
-11
.75       0
.0
-0
.12827     365
.76   0


u
n
i
t 7

c
o
m
='Left-Hand Side Half Vertical Boral Panel'

c
u
b
o
i
d          7  1   0
.0
-0
.0254     9
.5250
-9
.5250     365
.76   0
.

c
u
b
o
i
d          5  1   0
.0
-0
.12827    9
.5250
-9
.5250     365
.76   0
.

c
u
b
o
i
d          3  1   0
.0
-0
```

(continues on next page)

(continued from previous page)

```
u
n
i
t 8

c
o
m
='Empty Corner (Water)'

c
u
b
o
i
d          3  1   0
.12827   0       0
.12827      0         365
.76  0


u
n
i
t 10

c
o
m
='Top Boral/Basket Plate with water added to fit array dimensions'

c
u
b
o
i
d          5  1   9
.525
-9
.525
-0
.7754
-0
.87827    365
.76  0

c
u
b
o
i
d          7  1   9
.525
-9
.525
-0
.75
-0
.87827    365
.76  0
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d          3  1  11
.7500
-11
.75
-0
.75
-0
.87827    365
.76  0
.

c
u
b
o
i
d          4  1  11
.7500
-11
.75       0
.0
-0
.87827    365
.76  0
.

c
u
b
o
i
d          3  1  11
.87827
-11
.87827    0
.12827
-0
.87827    365
.76  0


u
n
i
t 11

c
o
m
='Bottom Boral/Basket Plate with water added to fit array dimensions'
```

(continues on next page)

```
c
u
b
o
i
d          5  1   9
.525
```

(continued from previous page)

```
c
u
b
o
i
d          7  1   9
.525
-9
.525     0
.87827   0
.75       365
.76  0

c
u
b
o
i
d          3  1  11
.7500
-11
.75      0
.87827   0
.75       365
.76  0
.

c
u
b
o
i
d          4  1  11
.7500
-11
.75      0
.87827   0
.0        365
.76  0
.

c
u
b
o
i
d          3  1  11
.87827
-11
.87827   0
.87827
-0
.12827    365
.76  0
```

(continues on next page)

```
u
n
i
t  12
```

(continued from previous page)

```
c
o
m
='Left-Hand Side Boral/Basket Plate with water added to fit array dimensions'

c
u
b
o
i
d          5  1   0
.87827   0
.7754     9
.525
-9
.525     365
.76  0

c
u
b
o
i
d          7  1   0
.87827   0
.75       9
.525
-9
.525     365
.76  0

c
u
b
o
i
d          3  1   0
.87827   0
.75      11
.75
-11
.75      365
.76  0
.

c
u
b
o
i
d          4  1   0
.87827   0
.0       11
.75
-11
.75      365
.76  0
.
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d           3  1   0
.87827
-0
.12827   11
.87827
-11
.87827   365
.76  0
.


u
n
i
t 13

c
o
m
='Right-Hand Side Boral/Basket Plate with water added to fit array dimensions'

c
u
b
o
i
d           5  1
-0
.7754
-0
.87827     9
.525
-9
.525    365
.76  0

c
u
b
o
i
d           7  1
-0
.75
-0
.87827     9
.525
-9
.525    365
.76  0
```

(continues on next page)

```
c
u
b
o
i
d           3  1
-0
```

(continued from previous page)

```
c
u
b
o
i
d          4  1   0
.0
-0
.87827    11
.75
-11
.75     365
.76  0
.

c
u
b
o
i
d          3  1   0
.12827
-0
.87827    11
.87827
-11
.87827  365
.76  0


u
n
i
t 20

c
o
m
='Top Boral/Basket Plate'

c
u
b
o
i
d          5  1   9
.525
-9
.525
-0
.7754
-0
.87827    365
.76  0

c
u
b
o
i
d          7  1   9
.525
-9
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d          3  1  11
.7500
-11
.75
-0
.75
-0
.87827    365
.76  0
.

c
u
b
o
i
d          4  1  11
.7500
-11
.75       0
.0
-0
.87827    365
.76  0
.


u
n
i
t 21

c
o
m
='Bottom Boral/Basket Plate'

c
u
b
o
i
d          5  1   9
.525
-9
.525     0
.87827   0
.7754     365
.76  0

c
u
b
o
i
d          7  1   9
.525
-9
.525     0
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d          3  1  11
.7500
-11
.75      0
.87827   0
.75       365
.76  0
.

c
u
b
o
i
d          4  1  11
.7500
-11
.75      0
.87827   0
.0        365
.76  0
.


u
n
i
t 22

c
o
m
='Left-Hand Side Boral/Basket Plate'

c
u
b
o
i
d          5  1   0
.87827   0
.7754     9
.525
-9
.525     365
.76  0

c
u
b
o
i
d          7  1   0
.87827   0
.75       9
.525
-9
.525     365
.76  0
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d          3  1   0
.87827   0
.75      10
.9999
-10
.9999    365
.76  0
.

c
u
b
o
i
d          4  1   0
.87827   0
.0       10
.9999
-10
.9999    365
.76  0
.


u
n
i
t 23

c
o
m
='Right-Hand Side Boral/Basket Plate'

c
u
b
o
i
d          5  1
-0
.7754
-0
.87827     9
.525
-9
.525    365
.76  0

c
u
```

(continues on next page)

```
b
o
i
d          7  1
-0
.75
-0
```

(continued from previous page)

```
c
u
b
o
i
d          3  1
-0
.75
-0
.87827    10
.9999
-10
.9999   365
.76  0
.

c
u
b
o
i
d          4  1   0
.0
-0
.87827    10
.9999
-10
.9999   365
.76  0
.



u
n
i
t 100

c
o
m
='17x17 Fuel Assembly in Basket'

a
r
r
a
y 1
-10
.7083
-10
.7083  0

c
u
b
```

(continues on next page)

```
o
i
d 3 1  11
 11 11
-11  365
.76  0
```

(continued from previous page)

```
c
u
b
o
i
d 0 1  11
-11  11
-11  365
.76  0

c
u
b
o
i
d 4 1  11
.75
-11
.75  11
.75
-11
.75  365
.76  0


u
n
i
t 101

c
o
m
='17x17 Fuel Assembly in Basket with Half Boral Panels'

a
r
r
a
y 2 0  0  0


u
n
i
t 112

c
o
m
='Top Row of Fuel Assemblies'

a
r
r
a
```

(continues on next page)

```
y 12
-47
.51308
12
.38154   0
```

(continued from previous page)

```
u
n
i
t 113

c
o
m
='Left Row of Fuel Assemblies'

a
r
r
a
y 13
-12
.38154
-47
.51308   0


u
n
i
t 114

c
o
m
='Bottom Row of Fuel Assemblies'

a
r
r
a
y 14
-47
.51308
-12
.38154    0


u
n
i
t 115

c
o
m
='Right Row of Fuel Assemblies'

a
r
r
a
y 15
-12
.38154
-47
.51308    0
```

(continues on next page)

(continued from previous page)

```
g
l
o
b
a
l
u
n
i
t 200

c
o
m
='Cask with 32 Fuel Assemblies'

a
r
r
a
y 3
-47
.51308
-47
.51308   0

c
y
l
i
n
d
e
r 3 1 87
.5  395
.76
-30

h
o
l
e 112   0       59
.89463  0

h
o
l
e 114   0
-59
.89463  0

h
o
l
e 113
-59
.89463  0        0
```

(continues on next page)

(continued from previous page)

```
h
o
l
e 115  59
.89463  0        0

h
o
l
e  20  59
.39136   48
.39136 0

h
o
l
e  20
-59
.39136   48
.39136 0

h
o
l
e  21  59
.39136
-48
.39136 0

h
o
l
e  21
-59
.39136
-48
.39136 0

h
o
l
e  22
-48
.39136   59
.39136 0

h
o
l
e  22
-48
.39136
-59
.39136 0

h
o
l
e  23  48
.39136  59
.39136 0
```

(continues on next page)

(continued from previous page)

```
h
o
l
e  23  48
.39136
-59
.39136 0

c
y
l
i
n
d
e
r 6 1 107
.5  425
.76
-60

c
u
b
o
i
d 0 1  108
-108  108
-108  425
.76
-60
end
 geom

read
 array

a
r
a
=1
n
u
x
=17
n
u
y
=17
n
u
z
=1

f
i
l
l 39
*1 2 2
*1 2 2
*1 2 8
*1 2 9
*1 2 22
*1 2 2
```

(continues on next page)

(continued from previous page)

```
 2
*1 2 2
*1 2 2
*1 2 38
*1 2 2
*1 2 2
*1 2 2
*1 2 2
*1 2 22
*1 2 9
*1 2 8
*1 2 2
*1 2 2
*1
 2 39
*1
end
 fill

a
r
a
=2
n
u
x
=3
n
u
y
=3
n
u
z
=1

f
i
l
l 8  4  8
     5 100 7
     8  6  8
end
 fill

a
r
a
=3
n
u
x
=4
n
u
y
=4
n
u
z
=1
```

(continues on next page)

(continued from previous page)

```
f
i
l
l
f101 end
 fill

a
r
a
=12
n
u
x
=4
n
u
y
=2
n
u
z
=1

f
i
l
l 101 101 101 101
      10  10  10  10
end
 fill

a
r
a
=13
n
u
x
=2
n
u
y
=4
n
u
z
=1

f
i
l
l 12 101
     12 101
     12 101
     12 101
```

(continues on next page)

(continued from previous page)

```
end
 fill

a
r
a
=14
n
u
x
=4
n
u
y
=2
n
u
z
=1

f
i
l
l  11  11  11  11
     101 101 101 101
end
 fill

a
r
a
=15
n
u
x
=2
n
u
y
=4
n
u
z
=1

f
i
l
l 101 13
     101 13
     101 13
     101 13
end
 fill
end
 array
read
 plot
```

(continues on next page)

(continued from previous page)

```
t
t
l
='2-d cross section of gbc-32 cask'

x
u
l
=
-90
y
u
l
=90
z
u
l
=100

x
l
r
=90
y
l
r
=
-90
z
l
r
=100

n
a
x
=800

u
a
x
=1
v
d
n
=
-1 end
end
 plot
read
 bounds

 xyf
=mirror
```

(continues on next page)

```
 end
 bounds
```

(continued from previous page)

```
end
 data
end
 kenova
end
```

11.5.5 Sample problem 5

Sample problem 5, listed in Listing 11.5, uses the CE 14 × 14 assembly design from problem 3, and performs a burnup-credit calculation using the horizontal burnup-profile option. The assembly configuration is taken to be a simple 2 × 2 assembly array with water reflection. This problem is only designed to illustrate the basic features of the horizontal profile option. In this example, it is assumed that there is a burnup gradient across the assemblies, such that half the fuel pins have a burnup exceeding the average assembly burnup by 10% and half the pins have a burnup of 10% less than the average, with the two burnup regions separated by the assembly diagonal. The input card required to simulate the two horizontal burnup regions in an assembly is

```
h
z
p
= 0
.9 1
.1 end
```

STARBUCS applies these factors to calculate compositions for each of the horizontally-varying burnup regions in each zone of the problem. It is important to note that the option inherently assumes that there is an equal volume/mass of fuel in each of the horizontal (or axial) zones since the code weights all regions equally when determining the average assembly burnup. To illustrate this, consider modeling an assembly with **only one quadrant** having a burnup that is 10% higher than the other three quadrants. The user would enter data for each of the four horizontal assembly quadrants or zones, e.g.,

```
h
z
p
= 0
.9766 0
.9766 0
.9766 1
.0700 end
```

such that the average of the HZP array entries is unity. This ensures that the average assembly burnup will be that specified in the power history data block. Note that this array is automatically normalized if NPR=yes (default). However, the user could substantially reduce the computational time involved by specifying only two fuel regions, e.g.,

```
h
z
p
= 0
.9766 1
.0700 end
```

and turning off the normalization option (e.g., NPR=no). The normalization option must be turned off to prevent the profile from being altered (since the sum is not equal to 2). This allows the user to account for the fact that, in this scenario, there are three quadrants having a lower burnup (and consequently three times the mass) and just one quadrant having an elevated burnup compared to the average. However, it is the responsibility of the user to ensure that the profiles and the KENO V.a problem description produce the desired average burnup.

In this sample problem the four assemblies are aligned so the lower burnup regions of the assemblies are adjacent to one another to maximize the system reactivity. The assembly geometry showing the different burnup regions of the assemblies is illustrated in Fig. 11.7. The criticality calculation is performed using the SCALE ENDF/B-VII continuous cross section library (CE_V7).

Following the STARBUCS calculation, the KENO V.a geometry model could be readily altered to simulate other assembly configurations (e.g., shuffle the fuel assembly locations). The CSAS5 case could subsequently be executed as a standalone case since all of the material compositions have already been created during the initial STARBUCS run. This facilitates the rapid evaluation of different fuel configurations without the need to regenerate the material compositions using STARBUCS.

Listing 11.5: STARBUCS input listing for sample problem 5

```
=starbucs

C
E 14
x14
a
s
s
e
m
b
l
y 4
x4
a
r
r
a
y
-
h
o
r
i
z
o
n
t
a
l
b
u
r
n
u
p
g
r
a
d
i
e
n
t
```

(continues on next page)

(continued from previous page)

```
c
e
_
v7
read
 comp
' UO2 Fuel Rod 3.038 wt %

u
o2  1
d
e
n
=10
.045  1  273
   92234 0
.027 92235 3
.038 92236 0
.014 92238 96
.921   end
'Zircalloy

a
r
b
m
z
i
r
c 6
.44 4 0 0 1 40000 97
.91 26000 0
.5 50116 0
.86 50120 0
.73 2 1 620  end
'Water

h2
o    3  1  end
end
 comp
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
s
q
u
a
r
e
p
i
```

(continues on next page)

(continued from previous page)

```
 end
end
 celldata
read
 control

a
r
p
=
c
e14
x14

n
a
x
=18

a
x
p
=
  0
.67053 0
.93322 1
.02433 1
.05329 1
.06026 1
.06185
  1
.06215 1
.06249 1
.06312 1
.06408 1
.06541 1
.06702
  1
.06836 1
.06760 1
.05918 1
.02515 0
.92262 0
.66935 end

n
h
z
= 2

h
z
p
= 0
.9 1
.1  end
```

(continues on next page)

```
n
u
c
```

(continued from previous page)

```
u
-234
u
-235
u
-236
u
-238
p
u
-238
p
u
-239
p
u
-240

p
u
-241
p
u
-242
a
m
-241
a
m
-242
m
a
m
-243
n
p
-237 end
end
 control
read
 hist

p
o
w
e
r
=28
.00
b
u
r
n
=520
.833
n
l
i
b
=2
d
o
w
```

(continues on next page)

(continued from previous page)

```
p
o
w
e
r
=28
.00
b
u
r
n
=520
.833
n
l
i
b
=2
d
o
w
n
=80  end

p
o
w
e
r
=28
.00
b
u
r
n
=520
.833
n
l
i
b
=2
d
o
w
n
=
-1865 end
end
 hist
read
 kenova
'*************************************************************
'* materials
'* 101 = uo2, lower axial region, low burnup region
'* 118 = uo2, upper axial region, low burnup region
```

(continues on next page)

(continued from previous page)

```
'* 201 = uo2, lower axial region, high burnup region
'* 218 = uo2, upper axial region, high burnup region
'* 2 = Zircaloy
'* 3 = Water
'*************************************************************
read
 param

t
m
e
=10000
g
e
n
=510
n
s
k
=10
n
p
g
=1000
end
 parm
read
 geom
'  Fuel Pin, Low Burnup Region

u
n
i
t           1

c
y
l
i
n
d
e
r   101  1  0
.484
-162
.53
-182
.85

c
y
l
i
n
d
e
r   102  1  0
.484
-142
.22
-162
.85
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   103  1  0
.484
-121
.90
-182
.85

c
y
l
i
n
d
e
r   104  1  0
.484
-101
.58
-182
.85

c
y
l
i
n
d
e
r   105  1  0
.484
-81
.27
-182
.85

c
y
l
i
n
d
e
r   106  1  0
.484
-60
.95
-182
.85
```

(continues on next page)

```
c
y
l
i
n
d
e
```

(continued from previous page)

```
c
y
l
i
n
d
e
r   108  1  0
.484
-20
.32
-182
.85

c
y
l
i
n
d
e
r   109  1  0
.484    0
.00
-182
.85

c
y
l
i
n
d
e
r   110  1  0
.484   20
.32
-182
.85

c
y
l
i
n
d
e
r   111  1  0
.484   40
.63
-182
.85

c
y
l
i
n
d
e
r   112  1  0
.484   60
.95
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   113  1  0
.484   81
.27
-182
.85

c
y
l
i
n
d
e
r   114  1  0
.484  101
.58
-182
.85

c
y
l
i
n
d
e
r   115  1  0
.484  121
.90
-182
.85

c
y
l
i
n
d
e
r   116  1  0
.484  142
.22
-182
.85

c
y
l
i
n
d
e
r   117  1  0
.484  162
.53
-182
.85
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   118  1  0
.484  182
.85
-182
.85

c
y
l
i
n
d
e
r   0    1  0
.4925 182
.85
-182
.85

c
y
l
i
n
d
e
r   2    1  0
.559  182
.85
-182
.85

c
u
b
o
i
d     3    1 4
p0
.7365 182
.85
-182
.85
'
'  Fuel Pin, High Burnup Region

u
n
i
t            2
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   201  1  0
.484
-162
.53
-182
.85

c
y
l
i
n
d
e
r   202  1  0
.484
-142
.22
-182
.85

c
y
l
i
n
d
e
r   203  1  0
.484
-121
.90
-182
.85

c
y
l
i
n
d
e
r   204  1  0
.484
-101
.58
-182
.85
```

(continues on next page)

```
c
y
l
i
n
d
e
```

(continued from previous page)

```
c
y
l
i
n
d
e
r   206  1  0
.484
-60
.95
-182
.85

c
y
l
i
n
d
e
r   207  1  0
.484
-40
.63
-182
.85

c
y
l
i
n
d
e
r   208  1  0
.484
-20
.32
-182
.85

c
y
l
i
n
d
e
r   209  1  0
.484    0
.00
-182
.85

c
y
l
i
n
d
e
r   210  1  0
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   211  1  0
.484   40
.63
-182
.85

c
y
l
i
n
d
e
r   212  1  0
.484   60
.95
-182
.85

c
y
l
i
n
d
e
r   213  1  0
.484   81
.27
-182
.85

c
y
l
i
n
d
e
r   214  1  0
.484  101
.58
-182
.85

c
y
l
i
n
d
e
r   215  1  0
.484  121
.90
-182
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   216  1  0
.484  142
.22
-182
.85

c
y
l
i
n
d
e
r   217  1  0
.484  162
.53
-182
.85

c
y
l
i
n
d
e
r   218  1  0
.484  182
.85
-182
.85

c
y
l
i
n
d
e
r   0    1  0
.4925 182
.85
-182
.85

c
y
l
i
n
d
e
r   2    1  0
.559  182
.85
-182
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d     3    1 4
p0
.7365 182
.85
-182
.85
'
'  2 x 2 Array of Lower Burnup Fuel Pins

u
n
i
t           3

a
r
r
a
y 1 3
*0
'
'  2 x 2 Array of Higher Burnup Fuel Pins

u
n
i
t           4

a
r
r
a
y 2 3
*0
'
'  Large Water Hole

u
n
i
t           5

c
y
l
i
n
d
e
r   3    1  1
.3140  182
.85
-182
.85
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r   2    1  1
.4160  182
.85
-182
.85

c
u
b
o
i
d     3    1 4
p1
.473  182
.85
-182
.85
'
'  Assembly 1 Unit

u
n
i
t           6

a
r
r
a
y      3
-10
.311
-10
.311
-182
.85

c
u
b
o
i
d     3    1 4
p11
.390  182
.85
-182
.85
'
```

(continues on next page)

(continued from previous page)

```
'  Assembly 2 Unit

u
n
i
t           7

a
r
r
a
y      4
-10
.311
-10
.311
-182
.85

c
u
b
o
i
d     3    1 4
p11
.390  182
.85
-182
.85
'
'  Assembly 3 Unit

u
n
i
t           8

a
r
r
a
y      5
-10
.311
-10
.311
-182
.85

c
u
b
o
i
d     3    1 4
p11
.390  182
.85
-182
.85
```

(continues on next page)

(continued from previous page)

```
'
'  Assembly 4 Unit

u
n
i
t           9

a
r
r
a
y      6
-10
.311
-10
.311
-182
.85

c
u
b
o
i
d     3    1 4
p11
.390  182
.85
-182
.85
'
'  Assembly Array (2 x 2)

g
l
o
b
a
l

u
n
i
t           10

a
r
r
a
y      7  3
*0

r
e
f
l
e
c
t
o
r  3  1 6
r30
.0  1
```

(continues on next page)

(continued from previous page)

```
end
 geom
read
 array

a
r
a
=1
n
u
x
=2
n
u
y
=2
n
u
z
=1
f
i
l
l
  1 1
  1 1  end
 fill

a
r
a
=2
n
u
x
=2
n
u
y
=2
n
u
z
=1
f
i
l
l
  2 2
  2 2  end
 fill

a
r
a
=3
n
u
x
=1
n
u
y
```

(continues on next page)

(continued from previous page)

```
  3 3 3 3 3 3 3
  3 5 3 3 3 5 4
  3 3 3 3 4 4 4
  3 3 3 5 4 4 4
  3 3 3 4 4 4 4
  3 5 4 4 4 5 4
  4 4 4 4 4 4 4   end
 fill

a
r
a
=4
n
u
x
=7
n
u
y
=7
n
u
z
=1
f
i
l
l
  3 3 3 3 3 3 3
  4 5 3 3 3 5 3
  4 4 4 3 3 3 3
  4 4 4 5 3 3 3
  4 4 4 4 3 3 3
  4 5 4 4 4 5 3
  4 4 4 4 4 4 4   end
 fill

a
r
a
=5
n
u
x
=7
n
u
y
=7
n
u
z
=1
f
i
l
l
```

(continues on next page)

(continued from previous page)

```
  4 4 4 4 4 4 3
  4 5 4 4 4 5 3
  4 4 4 4 4 3 3
  4 4 4 5 3 3 3
  4 4 3 3 3 3 3
  4 5 3 3 3 5 3
  4 3 3 3 3 3 3  end
 fill

a
r
a
=6
n
u
x
=7
n
u
y
=7
n
u
z
=1
f
i
l
l
  3 4 4 4 4 4 4
  3 5 4 4 4 5 4
  3 3 4 4 4 4 4
  3 3 3 5 4 4 4
  3 3 3 3 3 4 4
  3 5 3 3 3 5 4
  3 3 3 3 3 3 4  end


 fill
'

a
r
a
=7
n
u
x
=2
n
u
y
=2
n
u
z
=1
f
i
l
l
```

(continues on next page)

(continued from previous page)

```
  8 9
  7 6  end
 fill
end
 array
read
 bounds

 all
=void

 end
 bounds
end
 data
end
 kenova
end
```

11.5.6 Sample problem 6

The last sample problem uses KENO-VI to model a hexagonal VVER-440 fuel assembly. In this example the axial burnup profile is simulated using five axial regions of non-uniform volume (height). In this case the profile input in the AXP= array is not normalized by the code (i.e., NPR=NO). The criticality calculation is performed using actinide credit only. The input file is listed in Listing 11.6 and is the geometry is illustrated in Fig. 11.8.

Listing 11.6: STARBUCS input listing for sample problem 6

```
=starbucs

V
V
E
R
a
s
s
e
m
b
l
y
a
r
r
a
y

V7
-238
read
 comp
'UO2 Fuel

u
o2      1
d
e
n
=8
.7922 1
.0 293 92235 3
 3  92238 96
```

(continues on next page)

Fig. 11.7: Plot of the 2 x 2 array of CE 14 14 assemblies with burnup gradient.

(continued from previous page)

```
'Cladding

z
r  2
d
e
n
=6
.4073 1
.0  293  end
'Moderator

h2
o   3
d
e
n
=0
.71533 0
.9994 293 end

b
o
r
o
n   3
d
e
n
=0
.71533 0
.0006 293 end
end
 comp
'
read
 celldata

l
a
t
t
i
c
e
c
e
l
l
t
r
i
a
n
g
p
i
t
c
h
p
i
t
c
```

(continues on next page)

(continued from previous page)

```
end
 celldata
'
read
 control

a
r
p
=
v
v
e
r440
(3
.6
)
n
p
r
=
n
o

a
x
p
= 0
.652 0
.967 1
.084 0
.738 0
.462 end

n
u
c
=
u
-234
u
-235
u
-236
u
-238
p
u
-238
p
u
-239
p
u
-240

p
u
-241
p
u
-242
a
m
```

(continues on next page)

(continued from previous page)

```
end
 control
read
 hist

p
o
w
e
r
=35
.00
b
u
r
n
=1428
.6
d
o
w
n
=1826
n
l
i
b
=4 end
end
 hist
read
 keno
6
read
 param
 gen
=
1
1
0
 npg
=
1
0
0
0
 nsk
=
1
0
 end
 param
read
 geom

u
n
i
t  2
```

(continues on next page)

(continued from previous page)

```
c
o
m
='Vacant(water filled) hex'

h
e
x
p
r
i
s
m 10 0
.610 257
.0 0
.0

m
e
d
i
a 3 1 10

b
o
u
n
d
a
r
y 10

u
n
i
t   4

c
o
m
='UO2 Fuel Rod'

c
y
l
i
n
d
e
r 11 0
.386  14
.28 0
.0

c
y
l
i
n
d
e
r 12 0
.386  28
```

(continues on next page)

(continued from previous page)

```
c
y
l
i
n
d
e
r 13 0
.386 228
.44 0
.0

c
y
l
i
n
d
e
r 14 0
.386 242
.72 0
.0

c
y
l
i
n
d
e
r 15 0
.386 257
.00 0
.0

c
y
l
i
n
d
e
r 20 0
.455 257
.00  0
.0

h
e
x
p
r
i
s
m 30 0
.610  257
.00  0
.0
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a 101 1 11

m
e
d
i
a 102 1 12
-11

m
e
d
i
a 103 1 13
-12

m
e
d
i
a 104 1 14
-13

m
e
d
i
a 105 1 15
-14

m
e
d
i
a 2   1 20
-15

m
e
d
i
a 3   1 30
-20

b
o
u
n
d
a
r
y 30
```

(continues on next page)

(continued from previous page)

```
u
n
i
t  5

c
o
m
='UO2 Fuel assembly'

h
e
x
p
r
i
s
m 10 11
.800 257
.0 0
.0
r
o
t
a
t
e
a1
=
-30

a
r
r
a
y 1 10
p
l
a
c
e 12 12 1 3
*0
.0

b
o
u
n
d
a
r
y 10

g
l
o
b
a
l
u
n
i
t 1
```

(continues on next page)

(continued from previous page)

```
c
o
m
='UO2 assembly'

c
u
b
o
i
d 10  4
p15
.0  257
.0 0
.0

h
o
l
e 5
r
o
t
a
t
e
a1
=30

m
e
d
i
a 3  1 10

b
o
u
n
d
a
r
y 10
end
 geom
read
 array

c
o
m
='Assembly hexagonal rod array'

a
r
a
=1
t
y
p
=
h
e
```

(continues on next page)

(continued from previous page)

```
f
i
l
l
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2 4 4 4 4 4 4 4 4 4 4 4 2
2 2 2 2 2 2 2 2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 2
2 2 2 2 2 2 2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 2
2 2 2 2 2 2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2
2 2 2 2 2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2
2 2 2 2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2
2 2 2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2
2 2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2
2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2
2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2
2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2
2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2 2
2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2 2 2
2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2 2 2 2
2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2 2 2 2 2
2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2 2 2 2 2 2
2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2 2 2 2 2 2 2
2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 2 2 2 2 2 2 2 2
2 4 4 4 4 4 4 4 4 4 4 4 4 4 2 2 2 2 2 2 2 2 2
2 4 4 4 4 4 4 4 4 4 4 4 4 2 2 2 2 2 2 2 2 2 2
2 4 4 4 4 4 4 4 4 4 4 4 2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
end
 fill
end
 array
read
 bounds

 xyf
=reflect
 zfc
=water
 end
 bounds
end
 data
end
 keno
6
end
```

Fig. 11.8: Cutaway 3-D view of the hexagonal VVER assembly model with water hidden.

CHAPTER

TWELVE

SOURCERER: DETERMINISTIC STARTING SOURCE FOR CRITICALITY CALCULATIONS

D. E. Peplow, A. M. Ibrahim, K. B. Bekar, C. Celik, and B. T. Rearden

The Sourcerer sequence in SCALE deterministically computes a fission distribution and uses it as the starting source in a Monte Carlo eigenvalue criticality calculation. Using a reasonably accurate starting source, developed from the Denovo discrete-ordinates code through the DEVC sequence, Sourcerer improves the KENO/CSAS Monte Carlo calculation in two ways. First, the number of skipped generations required to converge the fission source distribution in the KENO solution is reduced. Second, for problems with loosely coupled fissionable areas, the reliability of the final eigenvalue (k_{eff}) is increased. Several convergence diagnostic capabilities available in the KENO codes help the user better measure when the fission source actually convergences.

12.1 Introduction

Monte Carlo eigenvalue calculations have been used in evaluating critical and sub-critical systems for decades. Calculations are typically done iteratively – starting with a set of fission neutrons, transporting them through the geometry until they leak or are absorbed, and then tabulating the fission sites for the next iteration. Each iteration corresponds to a generation in a chain reaction, and the eigenvalue, k_{eff}, is the ratio of the number of fissions in one generation to the number in the previous generation. Once the fission source distribution (the eigenfunction) has converged, many generations are simulated to obtain more estimates of k_{eff} with lower statistical uncertainty.

Two common questions that concern practitioners are (1) how many generations (skipped generations) are required before the fission source distribution is sufficiently converged that generational estimates of k_{eff} can be included in the final average of the eigenvalue (the active generations) and (2) has the fission source converged to the correct distribution, such that the final value of the eigenvalue will be correct? For most calculations, the final value of the k_{eff} eigenvalue is all that matters, so the convergence of the generational value of k_{eff} is used to determine the number of skipped generations. Fluxes and reaction rates computed during the active generations are more sensitive to the entire fission distribution and should only be accumulated when the fission distribution is sufficiently converged – which is not necessarily as soon as the generational value of k_{eff} has converged. To address this concern, tools such as Shannon entropy [Sha48] can be used to measure the convergence of the fission source distribution eigenfunction [UB03][UB05].

For the second question, the reliability in the final k_{eff} eigenvalue depends on whether the fission source converges to the correct distribution. Because no tool currently exists in SCALE to verify that the fission distribution is correct, models are often run for many generations using many histories per generation to ensure that the result does not change. Another approach to verify eigenvalue accuracy is to run several clones of the same problem, but each starting with different random numbers seed, and ensure that they all predict the same value for k_{eff}. Addressing this concern relies heavily on the engineering judgment of the practitioner.

Initial studies [IPW+11] have shown that the use of a starting fission distribution that is similar to the true fission distribution can both reduce the number of skipped generations required for fission source convergence and significantly improve the reliability of the final k_{eff} result. A recent study [Ibr13] focusing on criticality calculations of a spent

nuclear fuel cask showed that the chance of a low eigenvalue result due to undersampling from an unconverged source was dramatically reduced when using a deterministic starting source. In that study, a cask holding 24 assemblies was examined using a uniform starting source, a deterministic starting source with loose convergence criteria, and a deterministic starting source with tight convergence criteria. Multiple clones of KENO were run (with different random number seeds) for different values of skipped cycles. The number of clones that gave an incorrect result for k_{eff} was then tabulated. The results from that study, presented in Figure 2.4.1, show that using a deterministic starting source significantly increases the k_{eff} reliability.

The Sourcerer sequence in SCALE uses the solution from the Denovo [ESSC10] discrete-ordinates code (through the DEVC sequence) as that starting fission source distribution in a CSAS/KENO Monte Carlo [GPJD+11] calculation. For challenging criticality safety analyses, such as as-loaded spent nuclear fuel transportation packages with a mixed loading of low- and high-burnup fuel, even a low-fidelity deterministic solution for the fission source should be more accurate than the typical starting guesses of uniform or cosine shape over the fissionable regions. The Sourcerer sequence is fairly automated and uses an input very similar to standard CSAS (KENO V.a or KENO-VI) inputs, along with a short description of the mesh and other parameters for the Denovo calculation.

Fig. 12.1: Fraction of failure to agree with the reference k_{eff} value for KENO calculations with different starting sources (Figure 4 from Ref. 5).

12.2 Capabilities

The Sourcerer sequence calls a series of other sequences and utilities in SCALE – most importantly DEVC (for Denovo) and one of the CSAS sequences. Because DEVC can only use KENO-VI geometry, the utility c5toc6 geometry converter is used for KENO V.a geometries. The utility dso2msl is used to convert the Denovo spatial output (*.dso file) into a mesh source lite (*.msl) file that can be read as a starting source in KENO. All of the steps in Sourcerer are described in Table 12.1.

The sequence can be terminated at several points throughout the calculation using the "`parm=`" control on the "`=sourcerer`" line that starts the sequence. This capability can be used to stop the sequence between steps to ensure that the problem is progressing correctly or used to make a single source distribution that can be used with many variants of the final CSAS problem. Also when running several versions of a problem, if a file that is normally created by the Sourcerer sequence is supplied, then that step will be skipped, thus saving time. Note that files that use the name of the input file (*input*.inp) will be copied back to the user's working directory automatically when the

sequence finishes. Files that do not use the input file name can be copied back to the user's working area with an extra "=shell" directive in the *input*.inp input file.

The Sourcerer sequence can be used with KENO V.a or KENO-VI geometries. Either multi-group (MG) or continuous energy cross-section libraries can be used for the final CSAS calculation. Denovo only uses multi-group libraries, and self-shielding can be done like any MG sequence in SCALE. For efficient calculations, the user should understand the basics of Denovo eigenvalue calculations, how to use macromaterials, and how to use the KENO convergence metrics.

Table 12.1: Steps in Sourcerer for an input file named *input*.inp.

Step	Module/Task	Creates file	To stop after
0	Check user input		parm=check
1	c5toc6 – For KENO V.a sequences, the geometry is translated into KENO-VI geometry.	input.geom0...00.inp	
2a	Create Denovo input and AMPX cross sections	xkba_b.inp ft02f001 input.mmt	parm=deninp
2b	devc – Denovo eigenvalue calculation to compute a fission source distribution	*input*.dso	parm=denovo
3	dso2msl – Convert the fission source distribution file into a mesh source lite file	input.msl	
4a	Create the CSAS input		parm=csasinp
4b	csasX - Run the specific CSAS sequence using the mesh source lite as the starting source		

12.2.1 Using DEVC/Denovo

Some discussion is required about the extent and level of detail needed in the grid geometry that will be used in the Denovo calculation and the mesh-based starting source. When using discrete-ordinates transport (S:sub:*N*) methods alone for solving radiation transport problems, a good rule of thumb is to use mesh cell sizes on the order of a mean-free path of the particle. For complex problems, this could lead to an extremely large number of mesh cells, especially when considering the size of the mean-free path of the lowest energy neutrons.

In Sourcerer, the goal is to use the S_N calculation for a quick estimate. Accuracy is not paramount—just getting an approximation of the overall shape of the true fission source distribution will benefit the CSAS Monte Carlo calculation. With a more accurate starting source, fewer skipped generations may be required. At some point there is a time trade-off where calculating the starting source guess requires more time than the saved skipped generations would have used. Large numbers of mesh cells, as a result of using very small mesh sizes, for S_N calculations also use a great deal of computer memory.

Because the S_N calculation is only used to establish the initial distribution of source neutrons, the runtime and memory requirements for Sourcerer can be reduced by using larger/coarser mesh cell sizes than is typical for a stand-alone S_N analysis. Some general guidelines to consider when creating a mesh for the Denovo eigenvalue calculation/mesh-based starting source are as follows.

- All fissionable areas of the geometry and areas where neutrons can reasonably affect the eigenvalue should be included in the mesh.

- More detail should be used in the fissionable areas.
- Mesh planes should be placed at significant material boundaries.
- Neighboring cell mesh sizes should not be drastically different.

12.2.2 Convergence Metrics in KENO

KENO provides several tools that can be used to examine the convergence of k_{eff} and the fission source distribution. These include tools based on Shannon Entropy[1,3] and tools based on the mesh tally metrics described in [KS11]. Running Sourcerer should accelerate Shannon Entropy convergence for KENO calculations, and Sourcerer/KENO users should always check that the calculation Shannon Entropy has converged before active generations begin.

12.3 Sequence Input

The input file for a Sourcerer calculation is similar to a CSAS input, as shown in Table 12.2. There are two major differences between Sourcerer and CSAS: the beginning/end syntax of the CSAS input and the presence of the "read detSource" block for specifying the deterministic starting source. The CSAS input appears as one block in the Sourcerer sequence – instead of "=csasXX" use "read csasXX" and instead of "end data" use "end csasXX". If any parm= parameters are required for the CSAS sequence, they can be listed as "read csasX parm=(...)". Because Sourcerer runs both the DEVC and CSAS sequences, which will most likely use different cross-section data libraries (coarse group for S_N and fine group or continuous energy for Monte Carlo), the library for DEVC is listed in the new "read detSource" block, along with other parameters used by the Sourcerer sequence.

One important note about the geometry in Sourcerer is that for KENO V.a geometries, an outer boundary region should be added for an accurate internal conversion to a KENO-VI geometry prior to ray tracing. Also note that when using CSAS methods with the search capability, the Denovo mesh must encompass any changes to the size of the geometry.

Parameters used for building the deterministic starting source and establishing the CSAS sequence are specified in the detSource block. The library name for the Denovo calculation and the grid for the Denovo calculations are required. Many optional parameters are available for controlling the Denovo solver and applying boundary conditions (in the `eigenValParams` sub-block). The grid geometry is defined in a sub-block, or the keyword "`gridGeometryID=` *n*" can be used to point to a grid geometry defined in its own input block. The use of macromaterials to construct a more representative mesh model from the Monte Carlo geometry is controlled with the "`mmSubCell=`" and "`mmTolerance=`" parameters in the macromaterial sub-block.

The overall layout of the detSource block is shown in Table 12.3. The more common keywords for the eigenValParams sub-block are shown in Table 12.4 and Table 12.5. A full list of the Denovo parameters appears in Appendix A. Macromaterials are explained in detail in the DEVC manual, and a list of keywords is given in Table 12.6.

Table 12.2: Input file for a Sourcerer calculation (and differences with a CSAS input file, where black text is the same as CSAS and green text is new for Sourcerer sequence).

`=sourcerer parm=…`	Parm: check, deninp, denovo, csasinp

`read csasXX`
`Title for the problem`
`v7-252n`
	The CSASXX input (change "=csas" to "read csasXX")

`read xxx` `end xxx`	Standard CSAS blocks: composition, celldata, parameters (used for the final CSAS), geometry, array, and volume
`read bounds` `end bounds`	If the global unit is a simple cuboid, then any boundary conditions listed here are used to construct the Denovo input
`read start` `end start`	Ignored by Sourcerer - not used by the final CSAS A mesh-based starting source (nst=9) is created and supplied to CSAS
`read gridGeometry m` `end gridGeometry`	Mesh grids used by KENO for tallies, etc. (m is a user-assigned ID number)

`read xxx`
`end xxx`
`end csasXX`
	Other CSAS blocks: plot, x1ds, energy, biasing, importance, reactions, search, etc.
	End of CSASXX input (change "end data" to "end csasXX")

`read detSource`	
`dLibrary="…"`	Library name for Denovo (multi-group only)
`dParmString="…"`	Any parameters for the DEVC parm=() input

`gridGeometry n`
`…`
`end gridGeometry`
	Define a mesh grid that is used for the Denovo calculation
	OR

`gridGeometryID=m`	Reference a grid geometry defined above
`macromaterial`	Optional macromaterial information
`mmSubCells=3`	Number of rays per dimension to trace through at each voxel
`mmTolerance=0.1`	Tolerance for similar macromaterial volume fractions
`end macromaterial`	

`eigenValParams`
`…`
`end eigenValParams`
	Optional list of quadrature order, Legendre order, and other eigenvalue calculation parameters. Any boundary conditions listed here will override those from the bounds block.

`end detSource`	
`end data` `end`	

Table 12.3: The detSource block.

keyword	type	required	restrictions/comments
read detSource			
For the preliminary Denovo calculation			
dLibrary=	character	yes	multi-group library for Denovo calculation
dParmString=	character	no	any parameters for the DEVC parm=().
gridGeometry *id*		yes*	covers a cuboid where all points are in defined regions
title=	character		contained in double quotes (title="yada yada yada")
x planes … end	real array		adds list of *x* plane values (order not important)
x Linear *n min max*	int real real		adds *n*+1 *x* planes (*n* cells) evenly from min to max
y planes … end	real array		adds list of *y* plane values (order not important)
y Linear *n min max*	int real real		adds *n*+1 *y* planes (*n* cells) evenly from min to max
z planes … end	real array		adds list of *z* plane values (order not important)
z Linear *n min max*	int real real		adds *n*+1 *z* planes (*n* cells) evenly from min to max
tolerance=	real		for removing duplicate planes from *planes or *Linear
make3dmap			makes a *.3dmap file showing the grid geometry
xdivide=	integer	no	once all xplanes are entered, further divide them by this
ydivide=	integer	no	once all yplanes are entered, further divide them by this
zdivide=	integer	no	once all zplanes are entered, further divide them by this
end gridGeometry			
gridGeometryID=	integer	yes*	*either define a grid geoemtry in a sub block or refer to a grid geometry defined in its own block
macroMaterial		no	parameters for the macro material calculation to
…			create a more representative Denovo model
end macroMaterial			
eigenValParams		no	parameters for eigenvalue Denovo calculation, including
…			legendre=, quadrature=, tolerance=,
end eigenValParams			kTolerance=, etc.
end detSource			

Table 12.4: Common Denovo parameters in the eigenValParams sub-block.

keyword	type	default	restrictions/comments
eigenValParams			
quadType=	integer	2	0-level symmetric, 1-Gauss-Legendre product, 2-QR
legendre=	integer	0	P_L, L=highest Legendre polynomial, L=0,1,2,3,…
quadrature=	integer	8	level symmetric S_N quadrature, N=2, 4, 6, 8, 10, 12, 14, 16
polarsPerOct=	integer	2	Gauss-Legendre product quadrature or QR
azimuthsPerOct=	integer	2	Gauss-Legendre product quadrature or QR
diagnostics=	integer	0	0-no diganostics, 1-all diagnostics
output=	integer	0	0-no ouput, 1-all output
tolerance=	double	1.E-04	tolerance used in convergence test
toleranceMG=	double	1.E-04	tolerance used in convergence test
kTolerance=	double	1.E-05	tolerance on k
diagnosticLevel=	integer	0	0-off, 1-on
l2Tolerance=	double	0.01	tolerance on the L-2 norm
linfTolerance=	double	0.001	tolerance on L-inf
end eigenValParams			

Table 12.5: Boundary conditions in the eigenValParams sub-block.

keyword	type	default	restrictions/comments
eigenValParams			
xmin=	integer	0	boundary conditions on the six faces:
xmax=	integer	0	0 - vacuum
ymin=	integer	0	1 - reflective
ymax=	integer	0	2 - periodic
zmin=	integer	0	3 - white
zmax=	integer	0	(these will override the "read bounds" block if specified here.)
end eigenValParams			

Table 12.6: Macromaterial sub-block input.

keyword	type	length	default	restrictions/comments
macromaterial				
mmSubCell=	integer		1	rays per dimension to throw at each voxel
mmTolerance=	real		0.01	smallest volume fraction for macromaterial
mmSubCells	integer	6		rays per dimension to throw (x:ny,nz; y:nx,nz; z: nx,ny)
mmPointTest				use recursive bisection point testing method
mmRayTest				use ray tracing method
mmRTSpeed				optimize ray-tracing method for speed
mmRTMemory				optimize ray-tracing method for memory conservation
end macromaterial				

12.4 Sequence Output

In addition to the data contained in the main Sourcerer text output file, many other files are created containing the intermediate data used by the sequence. These files are listed in Table 12.7. Some of the files produced can be viewed using the Java Mesh File Viewer, which is distributed with SCALE.

Note that files that use the name of the input file (*input*.inp) will be copied back to the user's working directory automatically when the sequence finishes. Files that do not use the input file name can be copied back to the user's working area with an extra "`=shell`" directive in the *input*.inp input file.

Instructions on how to use the Java Mesh File Viewer to view the various output files listed in Table 12.7 as well as how to use the macromaterial table file are located in the DEVC manual and the Mesh File Viewer help file, which is accessible through the Help/Help menu.

Table 12.7: Files created by Sourcerer for an input file named *input*.inp.

Filename		Viewer	Description
Output Summary			
	input.out		main text output file, contains results summary
	input.msg		messages file
Geometry Conversion			
	i_c5toc6		input file for c5toc6 module
	input.geom000....inp		KENO-VI version of a KENO V.a geometry, if applicable
Denovo			
	i_devc		input file for DEVC sequence
	xkba_b.inp	V[a]	input file for Denovo – if this file is renamed to have a *.dsi extension (Denovo simple input), it is viewable in the Mesh File Viewer
	ft02f001		AMPX formatted cross sections for Denovo
	input.dso	V	Denovo fission source distribution
	input.mmt	V	macromaterial table, use with *.dso or *.dsi file
Mesh Source Conversion			
	i_util		input file for dso2msl utility
	input.msl	V	mesh source lite file, the starting source distribution
CSAS			
	i_csasXX		input file for the final CSASXX sequence
	input.fissionSource.3dmap	V	mesh tally of fission source distribution from KENO
	input.kenoNuBar.txt		text file containing value of nu-bar
[a]V – can be displayed with the Mesh File Viewer.			

12.5 Sample problems

In addition to the sample problems described in this section (with input files included with SCALE), the reader is referred to the paper by Ibrahim et al. for a detailed study using a real used nuclear fuel transport and storage canister containing assemblies with a range of initial enrichments and burnups.

12.5.1 Jezebel

Consider the Jezebel critical assembly [PU-MET-FAST-001 in Volume I of the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC(95)03, Organisation for Economic Co-operation and Development, Nuclear Energy Agency (OECD-NEA), September 2012]. This is a very simple problem (a single sphere) to solve with CSAS and can be useful as a way to demonstrate the Sourcerer sequence.

Input file

The standard CSAS inputs for Jezebel are shown below using both KENO V.a and KENO-VI geometries.

KENO V.a geometry

```
=csas5

J
e
z
e
b
e
l

v7
-252
n
read
 composition

p
u
-239 1 0 0
.037047   end

p
u
-240 1 0 0
.0017512  end

p
u
-241 1 0 0
.00011674 end

g
a     1 0 0
.0013752  end
end
 composition
read
 parameters

g
e
n
=110
n
p
g
=1000
n
s
k
=10
end
 parameters
read
 geometry

g
l
o
b
a
l
```

KENO-VI geometry

```
=csas6

J
e
z
e
b
e
l

v7
-252
n
read
 composition

p
u
-239 1 0 0
.037047   end

p
u
-240 1 0 0
.0017512  end

p
u
-241 1 0 0
.00011674 end

g
a     1 0 0
.0013752  end
end
 composition
read
 parameters

g
e
n
=110
n
p
g
=1000
n
s
k
=10
end
 parameters
read
 geometry

g
l
o
b
a
l
```

The above inputs can be easily changed into the following Sourcerer inputs (with geometry additions in brackets and extra Sourcerer input in braces).

KENO V.a geometry	KENO-VI geometry

{
=
s
o
u
r
c
e
r
e
r
}
 	
{read
}
 csas
5
 	
J
e
z
e
b
e
l
 	
v7
-252
n
read
 composition
 	
p
u
-239 1 0 0
.037047 end
 	
p
u
-240 1 0 0
.0017512 end
 	
p
u
-241 1 0 0
.00011674 end
 	
g
a 1 0 0
.0013752 end
end
 composition
read
 parameters
 	
g
e
n
=110
n
p
	{
	=
	s
	o
	u
	r
	c
	e
	r
	e
	r
	}
	
	{read
	}
	 csas
	6
	
	J
	e
	z
	e
	b
	e
	l
	
	v7
	-252
	n
	read
	 composition
	
	p
	u
	-239 1 0 0
	.037047 end
	
	p
	u
	-240 1 0 0
	.0017512 end
	
	p
	u
	-241 1 0 0
	.00011674 end
	
	g
	a 1 0 0
	.0013752 end
	end
	 composition
	read
	 parameters
	
	g
	e
	n
	=110
	n
	p

With either of these variations of the Jezebel problem, the fission source distribution can be tallied by KENO and saved to a mesh tally (*.3dmap) file by adding the following to the input:

```
read
 parameters

...

c
d
s
=1
end
 parameters

read
 gridGeometry

1

t
i
t
l
e
="Mesh for collecting fission source distribution"

x
L
i
n
e
a
r 28
-7
.0 7
.0

y
L
i
n
e
a
r 28
-7
.0 7
.0

z
L
i
n
e
a
r 28
-7
.0 7
.0
```

(continues on next page)

(continued from previous page)

```
end
 gridGeometry
```

Note that the mesh grid used for the KENO mesh tally can be different from the mesh grid used by Denovo to create a starting source in the Sourcerer sequence. Also note that more total histories (more particles per generation or more active generations) would be required to produce a KENO fission source tally with low relative uncertainties in every voxel.

Output file

The results for the standard CSAS calculations and the Sourcerer results are shown in Table 12.8 for calculations with the 252-energy-group and continuous-energy cross sections.

Table 12.8: Eigenvalue results for the Jezebel problem.

	Sample Problem	CSAS	Sourcerer
1.	KENO V.a geometry, v7-252	1.0045 ± 0.0017	1.0054 ±0.0018
2.	KENO-VI geometry, v7-252	0.9998 ± 0.0018	1.0007 ±0.0020
3.	KENO V.a geometry, ce_v7	1.0058±0.0027	1.0026 ±0.0017
3.	KENO-VI geometry, ce_v7	0.9990 ±0.0023	1.0041 ±0.0016

The Denovo fission source provides a reliable starting source that is similar to the actual fission source distribution computed by KENO (using `npg`=250000), as shown in Fig. 12.2.

Fig. 12.2: Fission source distribution from Denovo (left) and KENO (right).

Other variations

To increase the Denovo calculation speed (but decrease the fidelity of the fission source result), the discretization in angle (`quadrature=` or `polarsPerOct=/azimuthsPerOct=`) can be coarsened and/or the tolerance parameters can be loosened. To reduce the amount of memory required by Denovo, the number of Legendre moments in the scattering cross-section expansion can be reduced (`legendre=`). Using macromaterials can help increase the fidelity of the Denovo calculation with only a small increase in model setup time. Macromaterials do not impact the Denovo run time. Denovo diagnostic messages can be turned on and will print to the messages file.

Macromaterials (higher fidelity)	Looser tolerances (faster Denovo)
read detSource ... macromaterial mmSubCell=3 mmTolerance=0.001 end macromaterial end detSource	read detSource ... eigenValParams ... tolerance=1.0e-2 kTolerance=1.0e-3 end eigenValParams end detSource

Screen messages	Higher fidelity (slower Denovo)
read detSource ... e i g e n V a l p a r a m s ... d i a g n o s t i c s =1 o u t p u t =1 d i a g n o s t i c L e v e l	read sequence ... e i g e n V a l p a r a m s ... q u a d T y p e =2 p o l a r s p e r O c t =4 a z i m u t h s p e r O

CHAPTER

THIRTEEN

DEVC: DENOVO EIGENVALUE CALCULATION

Douglas E. Peplow and Cihangir Celik

13.1 Introduction

The DEVC (Denovo EigenValue Calculation) sequence is an interface to the Denovo discrete-ordinates package [ESSC10] for calculating criticality eigenvalue problems. This sequence reads an input file very similar to a CSAS6 input file [GPJD+11] that contains an extra block of input for describing the Denovo mesh grid and calculational parameters. Many of the subroutines are shared from the MAVRIC routines that interface with Denovo for fixed-source calculations.

This manual assumes that the user is familiar with the discrete-ordinates method for radiation transport and the Denovo package. DEVC provides an easy way for users to modify existing CSAS6 inputs and use them to run Denovo. The DEVC sequence also provides a way to create mesh geometry for Denovo from the combinatorial solid geometry description used by KENO-VI.

The steps in the DEVC sequence are listed in Table 13.1.

Table 13.1: Steps in DEVC for an input file named *input*.inp

Step	Module/Task	Creates file	To stop after
0	Check user input		
1	Self-shielding (celldata/cellm ix) calculations		
2	Produces optional *.png plots		
	Produces optional *.3mdap files (to visualize grid in MeshFileViewer)		`parm=check`
3	Creates AMPX cross sections for the "real" materials	`ft02f001`	`parm=cross`
4	Creates Denovo binary stream input file and the macromaterial table file	`xkba_b.inp` `input.mmt`	`parm=input`
5	Runs Denovo to compute k_{eff} and either the fluxes or the fission source	`input.dff` or `input.dso`	

The DEVC sequence uses KENO-VI geometry. Users can specify what output Denovo will generate: fluxes by space and energy in a binary *.dff (Denovo flux file) file or the space-only fission source distribution in a binary *.dso (Denovo spatial output) file. The eigenvalue is printed in the main output text file.

Some of the more common KENO starting source types are supported. Other starting source types may be added or extended to all of the different array types in the future. Currently, starting sources are not sent to Denovo because the Arnoldi solver does not use it. This may change in the future.

13.2 Sequence input

The input file for a DEVC calculation looks similar to a CSAS6 input file, as shown in Table 13.2. The major difference is that the parameter block contains information for the Denovo calculation, not the KENO Monte Carlo calculation. A macromaterial block is used to describe how the KENO-VI materials are mapped onto the Denovo mesh grid. Only multi-group cross-section libraries can be used with Denovo.

Table 13.2: Input file for a DEVC calculation (and differences with a CSAS6 input file, where black text is the same as CSAS6 and green text is new for DEVC sequence)

`=devc parm=…`	Parm: check, cross, input
`Title for the problem`	
`library`	Multi-group cross-section library name
`read xxx`	Standard CSAS6 blocks used by DEVC: composition, celldata, geometry, array, plot and gridGeometry.
`end xxx`	
`read bounds`	Bounds are used if the boundary of the global unit is a cuboid.
`end bounds`	
`read start`	Most KENO start types are supported for some array types. Currently, Denovo does not make use of a starting source.
`end start`	
`read xxx`	Not used by DEVC: volume, x1ds, energy, biasing, importance, reactions, and search
`end xxx`	
`read parameters`	Denovo discrete-ordinates parameters
`gridGeometry 7`	Mesh grid – list of planes in each dimension
`…`	
`end gridGeometry`	
`quadType=2`	
`polarsperoct=4`	List of quadrature order, Legendre order, upscatter, and other eigenvalue calculation parameters
`azimuthsperoct=4`	
`ktolerance=1.0e-5`	
`…`	
`xmin=0`	Boundary conditions – these override conditions listed in the bounds block
`…`	
`fissionSource`	Save fission source instead of fluxes
`end parameters`	
`read macromaterial`	How to create materials for each voxel in the mesh grid
`mmSubCell=3`	
`mmTolerance=0.001`	
`end macromaterial`	
`read xxx`	
`end xxx`	
`end data`	
`end`	

13.2.1 Parameters block

This block contains the parameters for the Denovo eigenvalue calculation, the grid geometry, and the macromaterials. Boundary conditions listed in the parameters block will override those listed in the bounds block (using CSAS6 syntax). Table 13.3 lists the Denovo calculation parameters and their default values, and Table 13.4 lists the keywords for the setting the boundary conditions and file saving options. The grid geometry is defined in a sub-block in the parameters block, or the keyword "`gridGeometryID=\ *n*\ `" can be used to point to a grid geometry defined in its own input block.

Table 13.3: Denovo parameters in the parameters block

keyword	type	default	restrictions/comments
read parameters			
discretization=	integer	4	0-diamond difference, 1-DD with flux fix-up:lin0, 2-theta-weighted DD, 3-linear discontinuous finite element, 4-step characteristics, 5-trilinear discontinuous finite element
quadType=	integer	2	0-level symmetric, 1-Gauss-Legendre product, 2-QR
legendre=	integer	3*	P_L, L=highest Legendre polynomial, L=0,1,2,3,… *default is to use min(the highest available in the data,3)
tportcorrection=	integer	1	transport correction: 0-none, 1-diagonal, 2-Cesaro *P_2 or higher is required for Cesaro
upScatter=	integer	1	upscatter iterations: 0-none, 1-yes, 2-ignore
xblocks=	integer	1	parallel calcs - how many divisions in x
yblocks=	integer	1	parallel calcs - how many divisions in y
zblocks=	integer	1	parallel calcs - how many commication layers in z
numSets=	integer	1	parallel calcs - how many energy sets
partUpscatter=	integer	1	partition upscatter (0-no, 1-yes)
quadrature=	integer	8	level symmetric S_N quadrature, N=2, 4, 6, 8, 10, 12, 14, 16
polarsPerOct=	integer	3	Gauss-Legendre product quadrature or QR
azimuthsPerOct=	integer	3	Gauss-Legendre product quadrature or QR
maxIters=	integer	1000	maximum number of iterations
diagnostics=	integer	0	0-no diganostics, 1-all diagnostics
output=	integer	0	0-no ouput, 1-all output
krylovSpaceSize=	integer	25	size in memory for Krylov space
tolerance=	double	1.E-04	tolerance used in convergence test
krylovType=	integer	0	0-GMRES, 1-BiCGStab
eigenSolver=	integer	1	0-power iteration, 1-Arnoldi, 2-shifted inverse
multiGSolover=	integer	1	0-Gauss-Seidel, 1-Krylov
withinGSolver=	integer	0	0-Krylov, 1-residual Krylov, 2-source iteration
mgSettings=	integer	0	0-user supplied, 1-automatic by Denovo
upGroupSolver=	integer	0	0-same as within-group solver, 1-Krylov, 2-residual Krylov, 3-source iteration, 4-single source iteration
acceleration=	integer	0	0-none, 1-two grid
maxItersMG=	integer	1000	maximum number of iterations
toleranceMG=	double	1.E-04	tolerance used in convergence test
keff=	double	1	starting guess of k
kTolerance=	double	1.E-05	tolerance on k
diagnosticLevel=	integer	0	0-off, 1-on
eigenSettings=	integer	0	0-user supplied, 1-automatic by Denovo
l2Tolerance=	double	0.01	tolerance on the L-2 norm
linfTolerance=	double	0.001	tolerance on L-inf
powerIterAcc=	integer	0	0-none, 1-rebalance, 2-RQI
arnoldiKSpace=	integer	25	
arnoldiRestarts=	integer	100	
calcMoments=	integer	1	0-off, 1-on
end parameters			

Table 13.4: Boundary conditions and what type of file to save

keyword	type	default	restrictions/comments
read parameters			
xmin=	integer	0	boundary conditions on the six faces:
xmax=	integer	0	0 - vacuum
ymin=	integer	0	1 - reflective
ymax=	integer	0	2- periodic
zmin=	integer	0	3 - white
zmax=	integer	0	(these will override the "read bounds" block if specified here.)
fluxes			save space/energy fluxes (default)
fissionSource			save the space-only fission source
end parameters			

13.2.2 Grid geometry block

Grid geometries ("`gridGeometry` *id*") require an identification number and then a description of a three-dimensional rectangular mesh by specifying the bounding planes of the cells in each of the *x*, *y*, and *z* dimensions. The keyword "`xPlanes ... end`" can be used to list plane values (in any order). The keyword "`xLinear` *n a b*" can be used to specify *n* cells between *a* and *b*. The keywords "`xPlanes`" and "`xLinear`" can be used together and multiple times – they will simply add planes to any already defined for that dimension. Any duplicate planes will be removed. Similar keywords are used for the *y* and *z* dimensions.

When using multiple instances of the keywords *``Linear`` and *``Planes`` for a given dimension, duplicates should be removed from the final list. In some cases, double precision math will leave two planes that are nearly identical but not removed (e.g., 6.0 and 5.9999999). To prevent this, a default tolerance is set to remove planes that are within 10^{-6} cm of each other. The user is free to change this by using the keyword "`tolerance=`" and specifying something else. Note that the tolerance can be reset to a different value in between each use of *``Linear`` or *``Planes``.

The keyword "`make3dmap`" for a particular grid geometry definition will create a file called "*outputName*.grid*id*.3dmap", which can be visualized using the Java Mesh File Viewer. These files will contain crude geometry information (unit, region, material) that corresponds to the center of each voxel.

Keywords for the grid geometry block are listed in Table 13.5.

Table 13.5: Grid geometry input keywords

keyword	type	restrictions/comments
read parameters		
gridGeometry *id*		covers a cuboid where all points are in defined regions
title=	character	contained in double quotes (title="yada yada yada")
x planes … end	real array	a list of *x* plane values (order not important)
x Linear *n min max*	int real real	adds *n*+1 *x* planes (*n* cells) evenly from min to max
y planes … end	real array	a list of *y* plane values (order not important)
y Linear *n min max*	int real real	adds *n*+1 *y* planes (*n* cells) evenly from min to max
z planes … end	real array	a list of *z* plane values (order not important)
z Linear *n min max*	int real real	adds *n*+1 *z* planes (*n* cells) evenly from min to max
tolerance=	real	for removing duplicate planes from *planes or *Linear
make3dmap		makes a *.3dmap file showing the grid geometry
xdivide=	integer	once all xplanes are entered, further divide them by this
ydivide=	integer	once all yplanes are entered, further divide them by this
zdivide=	integer	once all zplanes are entered, further divide them by this
end gridGeometry		
gridGeometryID=	integer	Either define a grid geoemtry in a sub block or refer to a grid geometry defined in its own block
end parameters		

13.2.3 Macromaterial block

In order to get more accurate solutions from a coarse-mesh discrete-ordinates calculation, Denovo can represent the material in each voxel of the mesh as a volume-weighted mixture of the real materials in the problem. When constructing the Denovo input, DEVC can estimate the volume fraction taken by each real material in each voxel by a sampling method. The user can specify parameters for how to sample the geometry. Note that finer sampling makes more accurate estimates of the material fraction but requires more setup time to create the Denovo input. Users should understand how the macromaterials are sampled and consider that when constructing a mesh grid. This is especially important for geometries that contain arrays. Careful consideration should be given when overlaying a mesh on a geometry that contains arrays of arrays.

Because the list of macromaterials could become large, the user can also specify a tolerance for how close two different macromaterials can be to be considered the same, thereby reducing the total number of macromaterials. The macromaterial tolerance, "`mmTolerance=`", is used for creating a different macromaterial from the ones already created by looking at the infinity norm between two macromaterials.

The number of macromaterials does not appreciably impact Denovo run time or memory requirements.

Keywords for the macromaterial block are listed Table 13.6. Two different sampling methods are available – ray tracing [IPE+09] with the keyword `mmRayTest` and point testing [Joh13] with the keyword `mmPointTest`.

Table 13.6: Macromaterial block input

keyword	type	length	default	restrictions/comments
read macromaterial				
mmSubCell=	integer		1	rays per dimension to throw at each voxel
mmTolerance=	real		0.01	smallest volume fraction for macromaterial
mmSubCells	integer	6		rays per dimension to throw (x:ny,nz; y:nx,nz; z: nx,ny)
mmPointTest				use recursive bisection point testing method
mmRayTest				use ray tracing method
mmRTSpeed				optimize ray-tracing method for speed
mmRTMemory				optimize ray-tracing method for memory conservation
end macromaterial				

Ray tracing

This method estimates the volume of different materials in the Denovo mesh grid elements by throwing rays through the KENO-VI geometry and computing the average track lengths through the each material. Rays are traced in all three dimensions to better estimate the volume fractions of materials within each voxel. The `mmSubCell` parameter controls how many rays to trace in each voxel in each dimension. For example, if `mmSubCell=` n, then when tracing rays in the z dimension, each column of voxels uses a set of $n \times n$ rays starting uniformly spaced in the x and y dimensions. With rays being cast from all three orthogonal directions, then a total of $3n^2$ rays are used to sample each voxel. One can think of subcells as an equally spaced sub-mesh with a single ray positioned at each center. The number of subcells in each direction, and hence the number of rays, can be explicitly given with `mmSubCells ny nz nx nz nx ny end` keyword for rays parallel to the x axis, y axis, and z axis. Fig. 13.1 shows different subcell configurations (in two dimensions) for a given voxel.

Ray tracing is a more robust method compared to the simple point testing method used in previous versions of SCALE/MAVRIC; however, it requires more memory than point testing. Ray tracing gives more accurate estimates of volume fractions because track lengths across a voxel give more information than a series of test points. Ray tracing is also much faster than point testing because the particle tracking routines are optimized for quickly determining lists of materials and distance along a given ray.

Ray tracing operates on the grid geometry supplied by the user and shoots rays in all three directions starting from the lower bounds of the mesh grid. An example of arbitrary assembly geometry is shown in Fig. 13.2. A ray consists of a number of steps that corresponds to crossing a different material along the path of the ray. Ratios of each step's length to the voxel length in the ray's direction determine the material volume fraction of that step in that voxel, and summation of the same material volume fractions gives the material volume fraction of that material in that voxel. Ray tracing through a single voxel that contains a fuel pin is illustrated in Fig. 13.3.

The final constructed macromaterials for this model are also shown in Fig. 13.2. Voxels that contain only a single material are assigned that original material number in the constructed macromaterials. For the voxels that contain a fuel pin with three different materials, the result is a new macromaterial consisting of the volume weighted fractions of each original material.

After the rays are shot in all three directions, the material volume fractions are updated and macromaterials are created by using these material volume fractions. Material volume fraction calculations for a single voxel, as shown in Fig. 13.3, are given by

$$F_m = \sum_{d=x,y,z} \sum_{r=1}^{N_r} \sum_{s=1}^{N_s} \begin{cases} \frac{L_{d,r,s}}{L_d}, & m_s == m \\ 0, & \text{otherwise} \end{cases} \qquad \text{and} \qquad V_m = \frac{F_m}{\sum_{n=1}^{N_m} F_n} \ ,$$

Fig. 13.1: Ray positions within a voxel with different mmSubCells parameters.

Fig. 13.2: Geometry model (left) and the Denovo representation (right) of an assembly using macromaterials determined by ray tracing.

where F_{m} = sampled fraction of material m in the voxel,

d = direction of the rays (x, y, z),

r = ray number,

N_{r} = total number of rays in the voxel for direction of d,

s = step number,

N_{s} = total number of steps for ray r in the voxel for direction of d,

$L_{\mathrm{d,r,s}}$ = length of the steps s for ray r in the voxel for direction of d,

$L_{\mathrm{d,}}$ = length of the voxel along direction of d,

m_{s} = material of step s,

m = material number,

N_{m} = total number of materials in the voxel, and

V_{m} = volume fraction of material m in the voxel.

Point testing

The recursive bisection method uses a series of point tests to determine the macromaterial fractions. For a given voxel, the material at the center is compared to the material at the eight corners. If they are all the same, the entire volume is considered to be made of that material. If different, the volume is divided into two in each dimension. Each subvolume is tested, and the method is then applied to the subvolumes that are not of a single material. When the ratio of the volume of the tested region to the original voxel becomes less than a user-specified tolerance (in the range of 10^{-1} to 10^{-4}), then further subdivision and testing are stopped. This is illustrated in Fig. 13.4.

In point testing, the keyword "`mmTolerance=f`" is interpreted to be where f is the smallest fraction of the voxel volume to consider. This same tolerance f is also used to limit the number of macromaterials. Before a new macromaterial is created, if one already exists where the fraction of each actual material matches to within the given tolerance, then

Fig. 13.3: Ray tracing (in two dimensions) through a voxel.

Fig. 13.4: Progression of the recursive bisection method (from upper left to lower right).

the existing material will be used. If using only a single point at the center of each voxel, use "`mmTolerance=1`". The `mmSubCell` keyword is not used in point testing.

Example

Fig. 13.5 shows an example of a cask geometry with two types of spent fuel (yellows), steel (blue), resin (green), and other metals (gray). When the Denovo geometry is set up by testing only the center of each mesh cell, the curved surfaces are not well represented (upper right). By applying the ray-tracing method and defining a new material made of partial fractions of the original materials, an improved Denovo model can be made. In the lower left of the figure, the Denovo model was constructed using one ray (in each dimension) per voxel and a tolerance of 0.1. This gives 20 new materials that are a mixture of the original 13 actual materials and void. With `mmSubCells=3` and an `mmTolerance=0.01`, 139 macromaterials are created.

A macromaterial table listing the fractions of each macromaterial is saved to a file called "*outputName*.mmt", where *outputName* is the name the user chose for his or her output file. This file can be used by the Mesh File Viewer to display the macromaterials as mixtures of the actual materials, as seen in lower row of Fig. 13.5. See the Mesh File Viewer help pages for more information on how to use colormap files and macromaterial tables.

13.2.4 Starting sources block

The default KENO-VI starting source is "flat over the volume specified by the unrotated, untranslated geometry record specified in the first position of the global unit boundary record in fissile material only". For DEVC, the default starting source strength is uniform in the fissile voxels contained within the bounding box of the global unit (uniform density). If macromaterials are used, the amounts in each voxel are volume averaged between fissile and non-fissile materials. Table 13.7 and Table 13.8 describe the starting sources available in the DEVC interface to Denovo.

Table 13.7: Starting source types (within the fissile areas of the listed shape)

	KENO-VI start type	DEVC
nst=0	the first surface of boundary (default)	The bounding box of global unit
nst=0	Within boundary of global array having a reflector key set to false	Not supported
nst=0	A cuboid defined by XSM, XSP, YSM, YSP, ZSM, and ZSP	Supported
nst=1	A cuboid defined by XSM, XSP, YSM, YSP, ZSM, and ZSP with cosine distributions	Supported
nst=2	Arbitrary fraction (FCT) in element NXS, NYS, NZS of the global array with the remainder in a cuboid defined by XSM, XSP, YSM, YSP, ZSM, and ZSP with cosine distributions	Supported for some array types (see Table 13.8)
nst=3	At the location TFX, TFY, TFZ in the element NXS, NYS, NZS of the global array	Supported for some array types (see Table 13.8)
nst=4	At the location TFX, TFY, TFZ in units NBX of the global array	Supported
nst=5	Across units NBX in the global array	Not supported
nst=6	List of points TFX, TFY, TFZ in global coordinates	Limited to 1 point
nst=6	List of points TFX, TFY, TFZ in element NXS, NYS, NZS of the global array	Limited to 1 point and only for some array types (see Table 13.8)
nst=7	Flat distributions in X and Y with [1-$\cos^2$(z)] in Z for a cuboid defined by XSM, XSP, YSM, YSP, ZSM, and ZSP	Supported
nst=8	Flat distributions in X and Y with a segmented distribution in Z for a cuboid defined by XSM, XSP, YSM, YSP, ZSM, and ZSP	Not supported
nst=9	Use a mesh source lite file	Not supported

Fig. 13.5: Cask geometry model (upper left) and the Denovo representation using (upper right) cell center testing. Representations using macromaterials determined by ray tracing are shown for (lower left) mmSubCell=1/mmTolerance=0.1 and (lower right) mmSubCell=3/mmTolerance=0.01.

Table 13.8: Supported array types for starting sources

no arrays	supported
cuboid	supported
hexagonal	supported
shexagonal	no
rhexagonal	no
dodecahedral	no

The starting source initialized in Denovo is always a volumetric source—DEVC does not create point sources (which would activate the first collision option in Denovo).

13.3 Sequence Output

The main text output file consists of the output from the cross-section processing codes and Denovo. The user should examine the output and pay attention to any warnings or errors. Table 13.9 lists the files generated during the DEVC sequence.

Table 13.9: Files created by DEVC for an input file named *input*.inp

Filename		Viewer	Description
Output Summary			
	input.out		main text output file, contains $k_{rm\text{eff}}$
	input.msg		messages file
Denovo			
	xkba_b.inp	V[a]	input file for Denovo – if this file is renamed to have a *.dsi extension (Denovo simple input), it is viewable in the Mesh File Viewer
	ft02f001		AMPX formatted cross sections for Denovo
	input.mmt	V	macromaterial table, use with *.dso or *.dsi file
	input.dff	V	Denovo fission fluxes
	input.dso	V	Denovo fission source distribution
[a]V – can be displayed with the Mesh File Viewer.			

13.3.1 Using the mesh file viewer

The Mesh File Viewer is a Java utility shipped with SCALE that is used for viewing mesh tallies from Monaco, as well as importance maps and mesh-based sources in MAVRIC. The Mesh File Viewer can be used with DEVC to view the Denovo input file (*.dsi, showing the starting source), the Denovo output fission source distribution (*.dso) file, or the Denovo output flux (*.dff) file.

With any Denovo file, material information for each voxel can be displayed. Users can use the graphical user interface to select colors for each material in the DEVC input and save them to a colormap text file (*.cmp) for later use. For example, Fig. 13.6 shows a cask model that has 13 materials with the default colors assigned by the viewer. A better color map (uranium is yellow, steel is blue, etc.) and an image using that color map are also shown in Fig. 13.6.

Fig. 13.6: Viewing material information with the Mesh File Viewer.

If the Denovo input was made using the mixed macromaterials, that can also be shown with the Mesh File Viewer. When one of the mesh files is loaded and the geometry is displayed (e.g., the materials for a cask model shown in Fig. 13.7), there will be many values since each macromaterial is treated by the Java viewer as a separate material. Redefining the color map using the GUI is not realistic.

A colormap needs to be defined for the original materials of the problem. For this example, there are 13 original materials, but when using macromaterials, 73 macromaterials are used in the discrete-ordinates model (as listed in the *.mmt file). The colormap file should only contain values for the 13 original materials. When loading the colormap, a corresponding *.mmt file can also be loaded. This will display mixed colors for the macromaterials, as shown in Fig. 13.7.

The final result is an image where the colors for the different values of the geometry attribute (which in the above example is material) are mixed in the ratio of the macromaterial definition.

13.3.2 Viewing the starting source

The Java MeshFileViewer (scale/cmds/meshview) can be used to visualize the Denovo binary stream input file to show materials and starting source strengths. An example is shown in Fig. 13.8.

Material Numbering

The cross sections produced by the SCALE cross-section mixing module ICE typically have a number of materials equal to the maximum material ID specified by the user in the "read composition" block. For a user input that contains materials 1, 3, and 5, the GIP-formatted cross-section file will contain five entries. For each lattice cell calculation that uses a cellmix= parameter, one more entry is contained in the GIP file. Hence, the GIP file does not contain the user's value from the "cellmix=" parameter but instead numbers the cellmix materials sequentially starting from 1+maximum(material ID). The Denovo geometry input and macroMixTable file produced by DEVC are modified to match the GIP cross-section file. When viewing the Denovo binary input file with the Mesh File Viewer, the GIP numbering for materials will be seen.

Fig. 13.7: Viewing material information from a Denovo input file.

Fig. 13.8: Fine-mesh version of sample problem 8, showing the materials using macromaterial blending of UO_2, MOX, clad, and water (left) and the starting source strength limited to cells with fissionable material (right).

13.4 Sample Problems

Sample problems have been made that correspond to the eight CSAS6 sample problems. In each problem, the KENO parameters block was commented out, a parameters block containing Denovo calculation parameters was added, and a grid geometry block was added. These sample problems use a coarse discretization and loose tolerances to obtain a short runtime. Users will typically use much finer discretization (mesh, quadrature) and higher fidelity parameter settings for real eigenvalue calculations. The voxelized geometry and starting source distribution are shown below in Fig. 13.9.

Results for the sample problems are displayed in `tab2-4a-10`. The sample problems used QR 1/1, a P_0 scattering expansion, a k tolerance of 0.001 and coarse meshes for speed. The higher fidelity runs used finer spatial meshes, default parameters of QR 2/2, P_0 scattering expansion, and the default k tolerance (10:sup:-5). Results for the longer-time CSAS6 and higher fidelity Denovo calculations are shown in Fig. 13.10.

Table 13.10: Sample problem results

	CSAS6						Denovo using DEVC			
	Short time			Long time			Sample problem		High Fidelity	
	k_{eff}	uncert	min	k_{eff}	uncert	min	k_{eff}	min	k_{eff}	min
1	1.0048	0.0023	1.94	1.00362	0.00018	380.18	0.889	10.97	1.00220	334.13
2	1.0048	0.0016	1.80	1.00421	0.00017	377.52	0.859	6.96	0.99816	245.34
3	0.9997	0.0017	0.45	0.99831	0.00018	178.69	0.982	3.30	0.99412	75.00
4	1.0013	0.0014	0.53	0.99841	0.00018	106.02	0.982	2.01	0.99412	30.91
5	0.9987	0.0019	0.46	0.99869	0.00020	63.18	0.982	1.40	0.99413	16.78
6	0.9998	0.0019	0.53	0.99830	0.00019	42.03	0.982	1.21	0.99412	8.98
7	0.9955	0.0017	1.43	0.99776	0.00019	101.56	0.882	8.98	0.99988	38.19
8	1.2668	0.0013	2.22	1.26784	0.00013	279.69	1.198	5.70	1.22295	204.08

Fig. 13.9: Denovo geometry (left) and starting source distribution (right) for the sample problems.

Fig. 13.10: Fission source distributions computed by CSAS6 (left) and Denovo (right).

CHAPTER

FOURTEEN

KMART5 AND KMART6: POSTPROCESSORS FOR KENO V.A AND KENO-VI

L. M. Petrie

KMART5 and KMART6 (**K**eno **M**odule for **A**ctivity-**R**eaction Rate **T**abulation) are modules whose primary purpose is to postprocess a KENO V.a or KENO-VI restart file with the corresponding working cross-section library to generate nuclide activity tables. It also allows collapsing and printing fluxes calculated by KENO. The KENO problem must have a mixing table, must calculate the fluxes, and must write a restart file containing the calculated data. KMART calculations are generally imbedded within a CSAS5 or CSAS6 input file immediately following the CSAS input as a stacked input case.

14.1 Introduction

KMART5 and KMART6 (**K**eno **M**odule for **A**ctivity-**R**eaction Rate **T**abulation) are modules whose primary purpose is to postprocess a KENO V.a or KENO-VI restart file with the corresponding working cross-section library to generate nuclide activity tables. It also allows collapsing and printing fluxes calculated by KENO. The KENO problem must have a mixing table, must calculate the fluxes, and must write a restart file containing the calculated data.

14.2 KMART Input Data

Input data for KMART is read into the program using free form blocked input similar to KENO. The data blocks are started with a READ *BLOCK NAME* and ended with an END *BLOCK NAME*. There are three data blocks that KMART can read. The first data block is named INITIAL, and the input starts with the keywords READ INITIAL. There are ten possible keyworded entries in this block that may be entered in any order.

Key-word	Variable	Description
PRTVOLS	PRINT_VOLUMES	A flag to cause the volumes calculated by KENO to be printed by KMART. Off by default, turn on by entering.
KU-NIT=	KUNIT	The logical unit number of the KENO restart file. The default is 35
FNI=	RESTART	*Mode_in* extra field in the input restart file name [restart_*mode_in*.keno_input] and [restart_*mode_in*.keno_calculated]. The default is an empty field.
XU-NIT=	XUNIT	The logical unit number of the cross-section library. The default is 4
ACT-BY-GRP	ACTIVI-TIES_BY_GROUP	A flag which turns on printing activities by group. If the fluxes are collapsed, the activities will be by broad group, otherwise they will be by fine group. Off by default, turn on by entering
RRPVOL	REAC-TION_RATES_PER_UNIT_VOLUME	A flag causing the activities to be printed per unit volume rather than integrated over the volume of the region. Off by default, turn on by entering
KENO3D	UNK3D K3DFILE	Unit number on which to write data for plotting with KENO3D. File name of the KENO input file (minus the trailing extension). The plot data file will be named K3DFILE.kmt.
NO-PRINT	PRINT_RESULTS	A flag allowing suppressing printing results.
FLUXBIN	FLUX_BIN	A flag to turn on generating a collapsed cross section file for TRITON.
WU-NIT	WGTD	The logical unit number on which to write an AMPX weighted library of the 1-D neutron cross sections.

A sample data block is given below.

```
R
E
A
D
I
N
I
T
I
A
L
K
U
N
I
T
=35
X
U
N
I
T
=4
E
N
D
I
```

(continues on next page)

```
N
I
T
I
A
L
```

(continued from previous page)

One of the next two blocks is required, but both can be specified if desired. If both are entered, either one can be first. The next data block specified is named ACTIVITY, and the input starts with the keywords READ ACTIVITY. It contains the data specifying which activities are to be calculated. The activities are specified by pairs of numbers giving the nuclide identifier and the reaction type identifier desired. A list of reaction types, also known as MT numbers, can be found in Appendix A of the XSLib chapter. These pairs are repeated until all the desired activities have been specified. If the nuclides are identified by the SCALE scheme, then the nuclide can be specified most explicitly by following the nuclide by the keyword MIX= and the mixture number the nuclide is in. By specifying a mixture of zero the activity will be calculated for each region in which the nuclide occurs. If the nuclide specifies a natural element identifier (1000*Z) and individual isotopes occur on the cross-section library, the isotope activities will be summed to produce the total activity for the element. If the nuclide is a special nuclide, i.e., identified with a prefix id times a million + a ZA, then MIX= must be specified as a mixture the nuclide occurs in. The data pair is described below.

Key-word	Variable	Description
	NUCLIDE	The nuclide identification number on the cross-section library for this activity request.
MIX	MIX-TURE	Mixture number of the nuclide for this activity request. This is an optional entry, and defaults to 0.
	REAC-TION	The reaction type identifier for this activity request.

If no activities are desired, then the block can be omitted. A sample block is given below.

```
R
E
A
D
A
C
T
I
V
I
T
Y 92235 18 92235 27 92235 1452
E
N
D
A
C
T
I
V
I
T
Y
```

The other input block is named COLLAPSE, and starts with the keywords READ COLLAPSE. There are two keyword entries that may be input in this block. A flux factor to normalize the fluxes by can be specified. It defaults to 1. The last fine group in the current broad group is the other entry. The broad groups are specified sequentially starting with group one. If the flux factor is specified more than once, the last value given is used. The data is specified as below.

Key-word	Variable	Description
FAC-TOR	FACTOR	A flux multiplier used to scale the fluxes before printing (default 1.0).
LASTG=	LAST_GROUP	The last fine group to be included in the current broad group. The broad groups are input sequentially starting with group one.

If no collapsed fluxes are desired, then the block can be omitted. A sample block is given below.

```
R
E
A
D
C
O
L
L
A
P
S
E
F
A
C
T
O
R 1
.0
L
A
S
T
G
=10
L
A
S
T
G
=20
L
A
S
T
G
=30
L
A
S
T
G
=56

E
N
D
C
O
L
L
A
P
S
```

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14.3 KMART Sample Input

Sample input data for KMART5 is given in Listing 14.1.

Listing 14.1: KMART5 sample input.

```
=kmart5
read
 initial
 kunit
=
6
4
 xunit
=
4
 prtvols
 end
 initial
read
 activity
1001 27
6012 27
8016 27
92235 18 92235 27 92235 1452
92238 18 92238 27 92238 1452
94238 18 94238 27 94238 1452
94239 18 94239 27 94239 1452
94240 18 94240 27 94240 1452
94241 18 94241 27 94241 1452
94242 18 94242 27 94242 1452
92000 18 92000 27 92000 1452
94000 18 94000 27 94000 1452
end
 activity
read
 collapse
 lastg
=
1
0
 lastg
=
2
0
 lastg
=
3
0
 lastg
=
5
6
```

(continues on next page)

(continued from previous page)

```
end
 collapse
end

end
```

CHAPTER

FIFTEEN

K5TOK6 AND C5TOC6: INPUT FILE CONVERSION PROGRAMS FOR KENO AND CSAS

15.1 Introduction

Program K5TOK6 can be used to automatically convert a KENO V.a input file to a KENO-VI input file. Program C5TOC6 can be used to automatically convert a CSAS5 input file to a CSAS6 input file. This functionality can be useful when converting a KENO V.a validation sequence to a KENO-VI validation sequence. It removes the problem of introducing a mistake or inadvertently changing the data when remodeling a geometry to the KENO-VI format. For some cases, however, the converted model may be a very inefficient KENO-VI model.

15.2 Description and Input Guide

Program K5TOK6 is a utility program that can be used to automatically convert a KENO V.a input file to a KENO-VI input file. Program C5TOC6 is a utility program that can be used to automatically convert a CSAS5 input file to a CSAS6 input file. For program K5TOK6, the "=KENOVA" record in the input stream is replaced by "=K5TOK6". The output file is then named _geom*nnnnnnn* where *nnnnnnn* is a unique 7-digit number. This allows a string of KENO V.a problems to be converted in one job. For program C5TOC6 the "=CSAS*BB*" record in the input stream (where the *BB* is 5, 25, or 2x) is replaced by "=C5TOC6 PARM=CSAS5." The output file is named _geom*nnnnnnn* where *nnnnnnn* is a unique 7-digit number.

For large problems, the output file may need to be edited to specify an increased value for parameter *NB8* in KENO-VI and also an increased value for parameter *DAB* in CSAS6. **The conversion makes no attempt to optimize the output file, so it almost surely will be inefficient in its use of storage, and in its use of bodies. This can lead to models that are very inefficient in their running time also.**

The input/output (I/O) units for K6TOK6 and C5TOC6 are given below. Note that K5TOK6 requires the cross-section library designated by the "LIB=" parameter in the KENO V.a input file.

Unit Number	Function
5	KENO V.a (or CSAS5) input file
6	Output
7	Input file generated for KENO-VI (or CSAS6)

Sample K5TOK6 input file is shown in Listing 15.1 and the corresponding converted KENO-VI input file is shown in Listing 15.2. Likewise, a C5TOC6 sample input file and corresponding converted CSAS6 input file are shown in Listing 15.3 and Listing 15.4, respectively.

Listing 15.1: Sample K5TOK6 problem.

```
=k5tok6
93
.2
%
u
o2
f2
h
/
u
-235
=337
read
 param



 npg
=
6
0
0
 fdn
=yes
 nub
=yes

 lib
=
4

 end
 param
read
 geom

c
u
b
o
i
d      1 1 2
p3
.81 2
p60
.325 25
.50 0

r
e
f
l
e
c
t
o
r   2 1 4
r
.312 0
.318 1
```

(continues on next page)

(continued from previous page)

```
c
u
b
o
i
d      0 1 2
p4
.128 2
p65
. 150
.
-1
.

c
o
r
e 0  1
-12
.384
-65
.
-29
.

c
y
l
i
n
d
e
r  0 1 142
.8 212
.
-60
.

c
y
l
i
n
d
e
r  3 1 144
.8 212
.
-62
.

c
u
b
o
i
d    0 1 275
.5
-638
.9 475
.
-744
.2 588
```

(continues on next page)

(continued from previous page)

```
r
e
f
l
e
c
t
o
r 4 1 5
r0
.32 1

r
e
f
l
e
c
t
o
r 5 1 5
r0 1
.27 1

r
e
f
l
e
c
t
o
r 3 1 5
r0
.64 1

r
e
f
l
e
c
t
o
r 0 1 5
r0 365 1

r
e
f
l
e
c
t
o
r 6 2 6
r5 6
```

(continues on next page)

(continued from previous page)

```
r
e
f
l
e
c
t
o
r 6 8 0 5 4
r0 6
end
 geom
read
 bias
 id
=
3
0
1

2

1
3
 end
 bias
read
 array
 nux
=
3
 nuy
=
1
 nuz
=
1
 end
 array
end
 data
end
```

Listing 15.2: Sample converted KENO-VI input file.

```
=kenovi
93
.2
%
u
o2
f2
h
/
u
-235
```

(continues on next page)

```
=337
```

(continued from previous page)

```
read
 param



 npg
=
6
0
0
 fdn
=yes
 nub
=yes

 lib
=
4

 end
 param
read
 geometry

u
n
i
t          1

c
u
b
o
i
d     1
               3
.810000
E
+00
-3
.810000
E
+00  6.032500E+01

-6
.032500
E
+01  2
.550000
E
+01  0.000000E+00

m
e
d
i
a     1    1       1
```

(continues on next page)

(continued from previous page)

```
v
o
l=  7.033051E+04

c
u
b
o
i
d     2
              4
.128000
E
+00
-4
.128000
E
+00  6.064300E+01

-6
.064300
E
+01  2
.550000
E
+01 -3.180000E-01

m
e
d
i
a     2    1       2
-1

v
o
l=  7.227070E+03

c
u
b
o
i
d     3
              4
.128000
E
+00
-4
.128000
E
+00  6.500000E+01

-6
.500000
E
+01  1
.500000
E
+02 -1.000000E+00
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a     0    1       3
-2
-1

v
o
l=  4.086382E+05

b
o
u
n
d
a
r
y     3

g
l
o
b
a
l

u
n
i
t          2

c
u
b
o
i
d     1
              1
.238400
E
+01
-1
.238400
E
+01  6.500000E+01

-6
.500000
E
+01  1
.220000
E
+02 -2.900000E+01
```

(continues on next page)

```
a
r
r
a
y     1       1
```

(continued from previous page)

```
p
l
a
c
e 1 1 1
-1
.23840
E
+01
-6
.50000
E
+01  -2.90000E+01

c
y
l
i
n
d
e
r   2
              1
.428000
E
+02  2
.120000
E
+02 -6.000000E+01

o
r
i
g
i
n
x
=  0
.000000
E
+00
y=  0.000000E+00

m
e
d
i
a     0    1       2
-1

v
o
l=  1.693890E+07

c
y
l
i
n
d
e
r   3
```

(continues on next page)

(continued from previous page)

```
                1
.448000
E
+02  2
.120000
E
+02 -6.200000E+01

o
r
i
g
i
n
x
=  0
.000000
E
+00
y=  0.000000E+00

m
e
d
i
a     3    1       3
-2
-1

v
o
l=  6.232560E+05

c
u
b
o
i
d     4
                2
.755000
E
+02
-6
.389000
E
+02  4.750000E+02

-7
.442000
E
+02  5
.880000
E
+02 -6.200000E+01

m
e
d
i
a     0    1       4
-3
-2
-1
```

(continues on next page)

(continued from previous page)

```
v
o
l=  7.065953E+08

c
u
b
o
i
d     5
              2
.755000
E
+02
-6
.389000
E
+02  4.750000E+02

-7
.442000
E
+02  5
.880000
E
+02 -6.232000E+01

m
e
d
i
a     4    1       5
-4
-3
-2
-1

v
o
l=  3.568000E+05

c
u
b
o
i
d     6
              2
.755000
E
+02
-6
.389000
E
+02  4.750000E+02
```

(continues on next page)

```
-7
.442000
E
+02  5
.880000
E
+02 -6.359000E+01
```

(continued from previous page)

```
m
e
d
i
a     5    1       6
-5
-4
-3
-2
-1

v
o
l=  1.415808E+06

c
u
b
o
i
d     7
              2
.755000
E
+02
-6
.389000
E
+02  4.750000E+02

-7
.442000
E
+02  5
.880000
E
+02 -6.423000E+01

m
e
d
i
a     3    1       7
-6
-5
-4
-3
-2
-1

v
o
l=  7.134720E+05

c
u
b
o
i
d     8
```

(continues on next page)

(continued from previous page)

```
                2
.755000
E
+02
-6
.389000
E
+02  4.750000E+02

-7
.442000
E
+02  5
.880000
E
+02 -4.292300E+02

m
e
d
i
a     0    1       8
-7
-6
-5
-4
-3
-2
-1

v
o
l=  4.069153E+08

c
u
b
o
i
d     9
                2
.805000
E
+02
-6
.439000
E
+02  4.800000E+02

-7
.492000
E
+02  5
.930000
E
+02 -4.342300E+02
```

(continues on next page)

```
m
e
d
i
a     6    2       9
-8
-7
```

(continued from previous page)

```
v
o
l=  3.316813E+07

c
u
b
o
i
d    10
               2
.855000
E
+02
-6
.489000
E
+02  4.850000E+02

-7
.542000
E
+02  5
.980000
E
+02 -4.392300E+02

m
e
d
i
a     6    3      10
-9
-8
-7
-6
-5
-4
-3
-2
-1

v
o
l=  3.380429E+07

c
u
b
o
i
d    11
               2
.905000
E
+02
-6
.539000
E
+02  4.900000E+02
```

(continues on next page)

(continued from previous page)

```
-7
.592000
E
+02  6
.030000
E
+02 -4.442300E+02

m
e
d
i
a     6    4      11
-10
-9
-8
-7
-6
-5
-4
-3
-2
-1

v
o
l=  3.444634E+07

c
u
b
o
i
d    12
               2
.955000
E
+02
-6
.589000
E
+02  4.950000E+02

-7
.642000
E
+02  6
.080000
E
+02 -4.492300E+02

m
e
d
i
a     6    5      12
-11
-10
-9
-8
-7
-6
-5
```

(continues on next page)

(continued from previous page)

```
v
o
l=  3.509453E+07

c
u
b
o
i
d    13              3
.005000
E
+02
-6
.639000
E
+02  5.000000E+02

-7
.692000
E
+02  6
.130000
E
+02 -4.542300E+02

m
e
d
i
a     6    6      13
-12
-11
-10
-9
-8
-7
-6
-5
-4
-3
-2
-1


v
o
l=  3.574874E+07

c
u
b
o
i
d    14
               3
.055000
E
+02
-6
.689000
E
+02  5.050000E+02
```

(continues on next page)

(continued from previous page)

```
-7
.742000
E
+02  6
.180000
E
+02 -4.592300E+02

m
e
d
i
a     6    7      14
-13
-12
-11
-10
-9
-8
-7
-6
-5
-4
-3
-2

-1

v
o
l=  3.640896E+07

c
u
b
o
i
d    15
              3
.055000
E
+02
-6
.739000
E
+02  5.050000E+02

-7
.742000
E
+02  6
.180000
E
+02 -4.592300E+02

m
e
d
i
a     6    8      15
-14
-13
-12
```

(continues on next page)

(continued from previous page)

```
-2
-1

v
o
l=  6.889984E+06

c
u
b
o
i
d    16
               3
.055000
E
+02
-6
.789000
E
+02  5.050000E+02

-7
.742000
E
+02  6
.180000
E
+02 -4.592300E+02

m
e
d
i
a     6    9      16
-15
-14
-13
-12
-11
-10
-9
-8
-7
-6
-5
-4

-3
-2
-1

v
o
l=  6.889856E+06
```

(continues on next page)

```
c
u
b
o
i
d    17
```

(continued from previous page)

```
                3
.055000
E
+02
-6
.839000
E
+02  5.050000E+02

-7
.742000
E
+02  6
.180000
E
+02 -4.592300E+02

m
e
d
i
a     6   10      17
-16
-15
-14
-13
-12
-11
-10
-9
-8
-7
-6
-5

-4
-3
-2
-1

v
o
l=  6.889984E+06

c
u
b
o
i
d    18
                3
.055000
E
+02
-6
.889000
E
+02  5.050000E+02
```

(continues on next page)

(continued from previous page)

```
-7
.742000
E
+02  6
.180000
E
+02 -4.592300E+02

m
e
d
i
a     6   11      18
-17
-16
-15
-14
-13
-12
-11
-10
-9
-8
-7
-6

-5
-4
-3
-2
-1

v
o
l=  6.889984E+06

c
u
b
o
i
d    19
              3
.055000
E
+02
-6
.939000
E
+02  5.050000E+02

-7
.742000
E
+02  6
.180000
E
+02 -4.592300E+02
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a     6   12      19
-18
-17
-16
-15
-14
-13
-12
-11
-10
-9
-8
-7

-6
-5
-4
-3
-2
-1

v
o
l=  6.889984E+06

c
u
b
o
i
d    20
               3
.055000
E
+02
-6
.989000
E
+02  5.050000E+02

-7
.742000
E
+02  6
.180000
E
+02 -4.592300E+02

m
e
d
i
a     6   13      20
-19
-18
-17
-16
-15
-14
```

(continues on next page)

(continued from previous page)

```
-7
-6
-5
-4
-3
-2
-1

v
o
l=  6.889984E+06

b
o
u
n
d
a
r
y    20
end
 geometry
read
 bias
 id
=
3
0
1

2

1
3
 end
 bias
read
 array
 nux
=
3
 nuy
=
1
 nuz
=
1
 end
 array
end
 data
end
```

Listing 15.3: Sample C5TOC6 problem.

```
=c5toc6    parm=csas5

s
a
m
p
l
e
p
r
o
b
l
e
m 1
c
a
s
e 2
c8
b
a
r
e

v7
-238
read
 composition

u
r
a
n
i
u
m  1
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end
end
 composition
read
 parameters

f
l
x
=
y
e
s
```

(continues on next page)

```
d
n
=
y
```

(continued from previous page)

```
end
 parameters
read
 geometry

u
n
i
t 1

c
y
l
i
n
d
e
r 1 1 5
.748 5
.3825
-5
.3825

c
u
b
o
i
d  0 1 6
.87
-6
.87 6
.87
-6
.87 6
.505
-6
.505
end
 geometry
read
 array

n
u
x
=2
n
u
y
=2
n
u
z
=2
f
i
l
l
f1 end
 fill
```

(continues on next page)

(continued from previous page)

```
end
 array
end
 data
end
```

Listing 15.4: Sample converted CSAS6 output file.

```
=csas26

s
a
m
p
l
e
p
r
o
b
l
e
m 1
c
a
s
e 2
c8
b
a
r
e

v7
-238
read
 composition

u
r
a
n
i
u
m  1
d
e
n
=18
.76 1 293 92235 93
.2 92238 5
.6 92234 1
.0 92236 0
.2 end
end
 composition
```

(continues on next page)

(continued from previous page)

```
read
 parameters

f
l
x
=
y
e
s
f
d
n
=
y
e
s
f
a
r
=
y
e
s
h
t
m
=
n
o
end
 parameters
read
 geometry

u
n
i
t          1

c
y
l
i
n
d
e
r   1
              5
.748000
E
+00  5
.382500
E
+00 -5.382500E+00

o
r
i
g
i
n
x
=  0
```

(continues on next page)

(continued from previous page)

```
m
e
d
i
a     1    1       1

v
o
l=  8.938970E+03

c
u
b
o
i
d     2
              6
.870000
E
+00
-6
.870000
E
+00  6.870000E+00

-6
.870000
E
+00  6
.505000
E
+00 -6.505000E+00

m
e
d
i
a     0    1       2
-1

v
o
l=  1.071004E+04

b
o
u
n
d
a
r
y     2

g
l
o
b
a
l
u
n
i
t         2
```

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```
c
u
b
o
i
d 1
                2
.748000
E
+01  0
.000000
E
+00  2.748000E+01
                0
.000000
E
+00  2
.602000
E
+01  0.000000E+00

a
r
r
a
y      1  1

p
l
a
c
e 1 1 1    6
.87000
E
+00   6
.87000
E
+00   6.50500E+00

b
o
u
n
d
a
r
y 1
end
 geometry
read
 array

n
u
x
=2
n
u
y
=2
n
u
z
```

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```
end
 array
end
 data
end
```

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