FUSION FOR ENERGY

REPORT

REPORT

ON

F4E-RADWASTE TOOL FOR ITER ANALYSES

Abstract

This document describes a tool and a methodology for analysing the activation and radwaste classification of nuclear systems exposed to neutron radiation such as ITER. The tool uses a 3D mesh to calculate and visualise various parameters related to radwaste generation and its classification including dose at 1 meter and contact dose rate. The methodology enables the automatic generation of radiological checklists. This document presents the application case of the methodology to the ITER 1D benchmark and discusses future developments and improvements.

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Subject:	**Methodology for radwaste assessment**		

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Table of Contents

Terms and Definitions

Term/Acronym	Definition
ACAB	Activation code
CDR	Contact Dose Rate
CSV	Comma-Separated Values
CuV	Cell-under-Voxel
D1S	Direct-one-step
D1SUNED	Patch for the MCNP code
F4E	Fusion for Energy
FMA-VC	Faible er Moyenne Activité à Vie Courte
FMESH	MCNP superimposed mesh
FOSS	Free and Open-Source Software
GUI	Graphical User Interface
GVR	Global Variance Reduction
GitHub	Online code repository
HPC	High Performance Computing
IAEA	International Atomic Energy Agency
ILW	Intermediate Level Waste
IO	ITER Organization
IRAS	Radiological Index for Disposal Acceptance
LLW	Low Level Waste
LMA	Limite Maximale d'Acceptabilité
MA-VL	Moyenne Activité à Vie Longue
MCNP	Monte Carlo N-Particles
PLY	Polygon File Format
R2S	Rigorous-two-step
R2SUNED	Activation code
STL	Standard Triangle Language
TFA	Très Faible Activité
UNED	Universidad Nacional de Educación a Distancia
VLLW	Very Low-Level Waste
VTK	Visualization Tool Kit, file format

Reference Documents

No.	Doc ID	Document title
[R1]	F4E_D_2THHJ9 v2.0	A. Cubí, SCtools, January 2022
[R2]	ITER_D_2RLM3G v1.1	G. Pedroche, E-lite 360º MCNP model - Model Report, April 2020
[R3]	ITER_D_YTFF2M v1.0	E. Polunovskiy, D1S_3.1.4-usermanual, July 2019
[R4]	N/A	X-5 Monte Carlo team, MCNP—A general Monte Carlo N-particle transport code, Version 5, Volume II: User's Guide, April 2003
[R5]	N/A	J. Alguacil, Propagation of statistical uncertainty in mesh-based R2S calculations, doctoral thesis in UNED 2021
[R6]	F4E_D_2NDMDR v2.1	N. Taylor, EXP-341-T3 support with radwaste assessments - D1 guideline for radwaste assessment of ITER systems and materials, October 2020
[R7]	N/A	IAEA Safety Standards Series no. GSG-1, Classification of Radioactive Waste, International Atomic Energy Agency, Vienna, 2009
[R8]	N/A	S. Rosanvallon et.al., Waste management within the framework of ITER in Cadarache, Fusion Engineering and Design 69 (2003) 531-536
[R9]	N/A	SURSPAMES020007 Indice F - Critères radiologiques d'acceptation des déchets TFA
[R10]	N/A	LOI n° 2006-739 du 28 juin 2006 de programme relative à la gestion durable des matières et déchets radioactifs. https://www.legifrance.gouv.fr/affichTexte.do?cidTexte=JORFTEXT000000240700
[R11]	ITER_D_4LGZZY v3.3	J. Wang, ITER Type A radwaste management plan – Interfaces with external facilities, November 2022
[R12]	N/A	D. Torcy, private communication, May 2023
[R13]	N/A	J. Sanz et al., ACAB. Inventory code for nuclear applications: User's Manual V. 2008, NEA-1839. December 2008
[R14]	ITER_D_QPUHZL v1.3	T. David, Checklist for radwaste inventories, June 2015
[R15]	N/A	https://github.com/Radiation-Transport, April 2023
[R16]	N/A	N. Taylor, private communication, June 2023
[R17]	F4E_D_2LYKL7 v1.1	R. Pampin, Approximate analytical formulations for gamma dose rates from unscattered activation sources, June 2020

1. Introduction

1.1. Scope and purpose

This document introduces and describes the F4E-Radwaste tool and methodology, designed, and built to automate the analysis of nuclear systems exposed to neutron radiation from the perspective of activation and radwaste management. The tool employs a fine 3D mesh to calculate radwaste-related parameters for the system and, in addition to the visualisation capabilities provided by such approach, it can be used to evaluate the classification of radwaste packages and to generate radwaste checklists.

The purpose of this document is to explain the principles of the radwaste regulations applicable to ITER, describe how the F4E-radwaste methodology works, and serve as a user manual for the tool. It includes all the necessary satellite software codes and processes required for the use of F4E-Radwaste and provides detailed explanations of how to use the tool effectively. The application of the methodology to the ITER 1D benchmark is presented as an example, and the results and implications are briefly discussed.

The determination of the radwaste parameters and classification of the components of a system that undergoes a process of neutron induced nuclear activation requires a complex multi-step approach coupling neutron transport and activation physics models and analysis tools. The methodology to perform the calculation is usually based on a per-component basis. The F4E-Radwaste methodology has been designed to streamline the radwaste calculation process and to provide results in a super-imposed mesh basis. Obtaining results in a fine 3D mesh allows the analyst to optimize the radwaste packaging strategy to minimize the amount of material classified with a high radwaste class level. This may translate into economic and operational advantages as higher radwaste class levels involve stiffer regulations.

1.2. Features

The F4E-Radwaste tool offers a range of powerful features that enable it to accurately calculate radwaste-related parameters and provide valuable insights into the behaviour of activated systems. These features include:

1.2.1. Fine 3D mesh and per-component basis

F4E-Radwaste employs a fine 3D mesh superimposed on the geometry of the system under study to calculate radwaste-relevant parameters, such as total activity, radionuclide inventory, IRAS and radwaste class. The tool can also provide these results on a per-component basis, allowing users to identify which specific components are contributing the most to the radwaste classification. Furthermore, the per-component basis allows the automatic generation of radwaste checklists, which greatly benefits from employing other F4E nuclear analysis workflows, especially during the MCNP input preparation [R1].

1.2.2. Package definition

F4E-Radwaste can also generate radwaste classifications for arbitrarily defined radwaste packages. Users can define the size, location, and materials included in each package, and the tool will calculate the relevant radwaste parameters for them. This allows users to determine the most appropriate methods for the disposal or treatment of each package.

1.2.3. Compatibility with complex radiation transport models

F4E-Radwaste can work well with the most complex radiation transports models like the latest 360-degree tokamak ITER model, E-Lite [R2]. During all the steps of the process, the methodology follows the cell-under-voxel (CuV) approach, [R3], enabling it to correctly transport radiation and record results over the 3D mesh while considering each material present in the voxel independently.

1.2.4. 3D Graphic User Interface

The last steps of the analysis process are performed using an easy-to-use 3D graphic user interface (GUI). The GUI allows users to interactively manipulate and visualize the results and permits the interactive definition of radwaste packages on-the-fly. This streamlines the analysis process and makes it more accessible to users who may be not proficient with programming workflows.

1.3. System requirements

The F4E-Radwaste methodology is a multi-step process that requires three different software programs used in sequence:

1. MCNP5 [R4] with the D1SUNED3.1.4 [R3] patch applied (for neutron transport only),
2. R2SUNED [R5]
3. F4E-Radwaste tool

The F4E-Radwaste methodology first steps (employing MCNP and R2SUNED) can be computationally intensive when dealing with complex geometries and/or big superimposed meshes. Therefore, it is recommended to perform them in a supercomputer that allows the parallel use of several nodes and computer cores (HPC). The HPC systems usually employ a Linux operating system. The installation and requirements of the MCNP5 + D1SUNED is out of the scope of this document. The installation of R2SUNED, however, will be explained for a Linux machine. Newer versions of D1SUNED may be incompatible with the R2SUNED code or the F4E-Radwaste tool. Future developments of the F4E-Radwaste may solve compatibility issues.

The F4E-Radwaste tool requires far less computation resources and therefore it is intended to be installed and used in a personal workstation or laptop, not in a HPC system. The F4E-Radwaste tool requires the Windows operating system and a Python 3.11 distribution. The amount of RAM required to run the tool depends on the complexity of the model and the size of the superimposed mesh, but 8 GB of RAM should suffice for most applications, with 16 GB or more recommended for larger models. It is recommended that the F4E-Radwaste tool is displayed in a monitor with a native 1920x1080p resolution. Different resolutions will also work but the scaling of the text font may cut the messages of certain buttons.

1.4. License

The F4E-Radwaste tool was developed in-house and is licensed under the EUPL, Version 1.2 or (as soon they will be approved by the European Commission) subsequent versions. You may not use this work except in compliance with the Licence. Unless required by applicable law or agreed to in writing, software distributed under the Licence is distributed on an “AS IS” basis, WITHOUT WARRANTIES OR CONDITIONS OF ANY KIND, either express or implied.

2. Radwaste classification in ITER

2.1. Classification overview

The ITER operation will produce high levels of neutron flux throughout the tokamak, and particularly inside the vacuum vessel. When neutrons are transported through the reactor geometry and systems, they interact with its components, inducing nuclear activation. Hundreds of different radioisotopes are generated in the activation process and many of them have long half-lives. Long-lived isotopes will remain active at the end-of-life and decommissioning of the reactor and will lead to some components being declared as radioactive. Radioactive components have special requirements regarding their management, handling, treatment, storage, transportation, and ultimate disposal [R6].

There are classifications schemes to distinguish between the requirements of the components depending on the type of radiation and the intensity of the source. The IAEA proposes a system that divides the radwaste between six classes but does not specify radwaste classification rules to assign to a component one of those classes [R7]. As ITER is under the French regulations, it will use the French radwaste classification system [R8]. There are three radwaste classes relevant to ITER according to the French regulations (from low to high level):

- **TFA** (Très Faible Activité). It is the counterpart of the Very Low-Level Waste (VLLW) class proposed by the IAEA. This type of radwaste can be buried at shallow depth.
- **FMA-VC** (Faible et Moyenne Activité à Vie Courte). It is the counterpart of the Low-Level Waste (LLW) class proposed by the IAEA. It corresponds to low to medium activity of isotopes with a half-life usually below 31 years. It is also known as **Type A**; this document will use Type A from now on.
- **MA-VL** (Moyenne Activité à Vie Longue). It is the counterpart of the Intermediate-Level Waste (ILW) class proposed by the IAEA. It corresponds to medium activity of isotopes with a long half-life. It is also known as **Type B**; this document will use Type B from now on.

2.2. Classification criteria

To assign a radwaste class to a batch of waste, the activation parameters of the batch are first compared against the criteria of the lowest class. If the criteria of the lowest class are not met, the process is repeated with the next higher class until the criteria of a class are met and the batch can be assigned to that class.

2.2.1. TFA criteria

A batch of waste fulfils the TFA criteria if its IRAS parameter is ≤ 1.0. If a batch is composed of several packages, any of the packages could have IRAS values ≤ 10.0 if the average IRAS of the whole batch remains below 1.0. The IRAS (Radiological Index for Disposal Acceptance) is calculated as:

$$\mathrm{IRAS} = \sum_{i=1}^{n} \frac{A_i}{10^{C_i}}$$

Where A_i is the specific activity in Bq/g of nuclide i and C_i is the TFA waste class, a number defined as 0, 1, 2 or 3 depending on the isotope [R9].

2.2.2. Type A criteria

The criteria for Type A are that no isotope present in the material should exceed its LMA (Limite Maximale d'Acceptabilité). The LMA is an activity limit in Bq/g that is specific for each isotope.

2.2.3. Type B criteria

If a package has failed to meet, first: the TFA criteria, and second: the Type A criteria, it gets classified as Type B immediately. While [R10] specifies more criteria to classify packages with classes higher than Type B, Type B is the highest radwaste class relevant for ITER and therefore F4E-Radwaste will not apply further checks once a package reaches Type B classification.

2.3. Dose rate

Information on the dose rates of the components and radwaste packages is relevant due to the requirements of the manipulation and transport operations.

The components have dose rate limit of 100 μSv/h over which they cannot be manually handled. If a Type A component or package dose rate exceeds this limit, remote handling is required, otherwise the component would be disposed as if it had a Type B classification, [R11].

A value of 2 mSv/h at the surface is the limit for a Type A package transport. If a Type A package exceeds 2 mSv/h it would need to be transported as a Type B package, [R12].

3. Process description

This section presents an explanation on the flow of data and the different calculations and post-processing steps performed with the F4E-Radwaste methodology. See Figure 1 for an overview schematic of the whole process. It is divided in 4 main steps:

1. Neutron transport calculation.
2. Activation calculation.
3. Post-processing.
4. Visualization and package definition.

In all the 4 steps a superimposed CuV mesh-based approach is followed. Both the geometry of the system and the parameters of the mesh of study are defined at the model specification file that is provided as input in the neutron transport calculation. Throughout the rest of the process, those mesh parameters will remain the same.

To obtain the radwaste classification of radwaste packages first a neutron transport calculation is performed to obtain the neutron flux and spectra distributions throughout the mesh. With this neutron data, an irradiation scenario and material data an activation calculation is performed to obtain the specific activity of every isotope. The results of the previous steps are then post-processed to be able to apply the radwaste classification criteria

to them. In a final step, the results are organized into radwaste packages for which a radwaste class is assigned in an interactive workflow that allows the analysis and optimization of the packaging strategy on the fly.

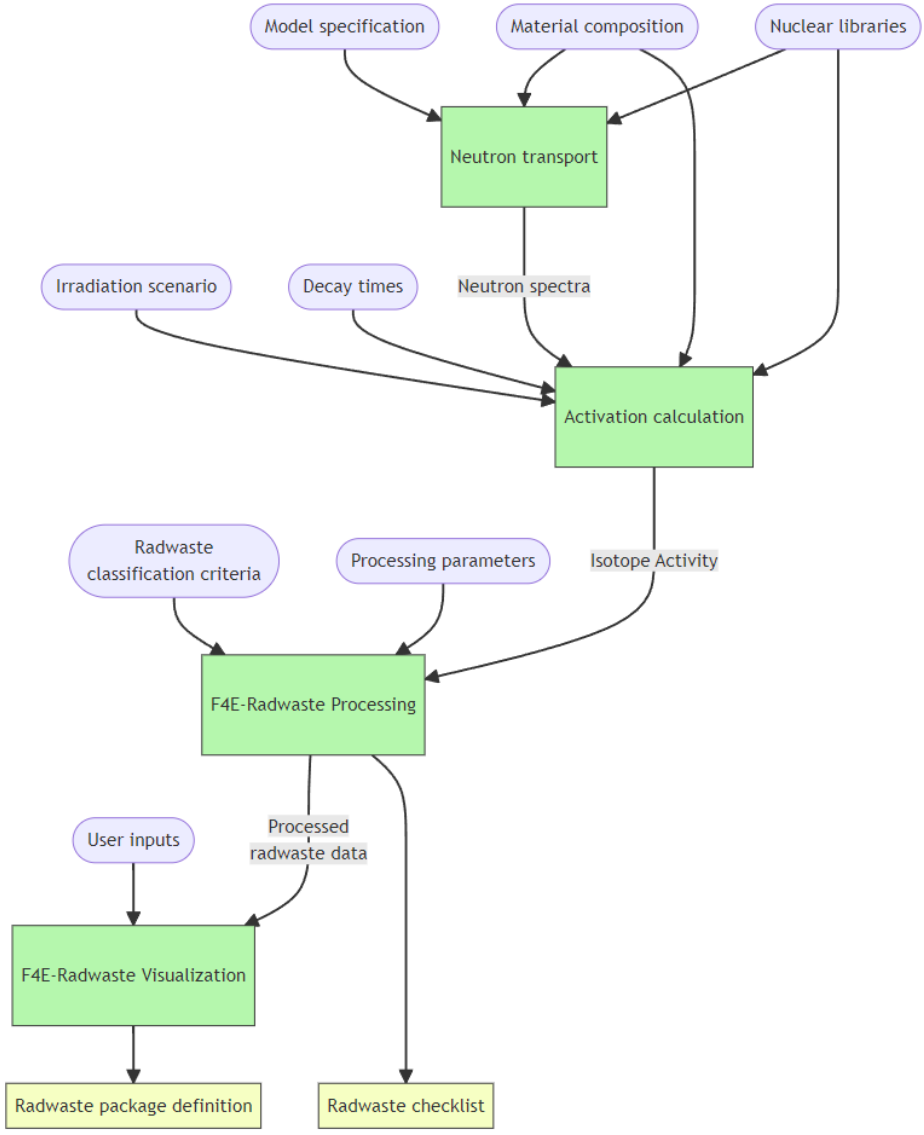


Figure 1 - F4E-Radwaste methodology flow diagram

3.1. CuV method

Recording results of a Monte Carlo radiation transport simulation in a mesh superimposed (i.e. non-conformal) to the geometry usually produces a biasing effect. This bias appears at the mesh cells (voxels) that contain more than a single material. Even if two components share the same material composition but with a different density, the bias will be present. The bias is especially important at the border of a material with empty space or a very low-density material like air.

The composition and density of the material occupying a space influences the radiation transport. High density and radiation absorbing materials produce shielding that reduces the ability of the particles to be transported through them. In a voxel containing a combination of high-density and low-density materials, it is common to observe higher particle fluxes in the lower density materials. While the transport of the particles correctly considers the transition between materials, the result recorded on a voxel consists in a single value, the average of the nuclear response of all the materials contained in the voxel. When studying a component, this usually translates into incorrectly higher particle fluxes recorded at the component's borders.

The CuV approach [R3] avoids this biasing effect by recording an independent value for each material contained inside every voxel. During all the steps of the F4E-Radwaste methodology the CuV approach is

used. Concretely, the CuV used here provide results that are independent for each of the different MCNP cells present in every voxel. Even if two components share the same density and material composition, and appear in the same voxel, an independent result will be considered for each of them.

3.2. Neutron transport

In the first step of the methodology a neutron transport simulation is performed to obtain the neutron flux and spectra throughout the superimposed mesh. The neutron transport simulation is done stochastically via the Monte Carlo method. Monte Carlo is the preferred and most common approach for nuclear analysis in the ITER context. The complexity of the ITER tokamak model and the level of intricacy of its systems makes deterministic calculations unfeasible.

The software code employed for the neutron transport is the MCNP5 [R4]. While many Monte Carlo codes exist, MCNP is the only practical option due to the technical requirements of the ITER analysis and the confidence in it by the relevant organizations like IO and the nuclear regulator. Moreover, the F4E nuclear team and its suppliers have extensive experience with this software. However, vanilla MCNP has proven ineffective to deal with the level of complexity of the most up-to-date, detailed, and extensive (360-degree) ITER models [R2] in terms of memory handling and runtime. It is necessary to apply a patch that improves its performance and adds new and valuable functionalities like the CuV approach. The D1SUNED3.1.4 [R3] patch of MCNP5 is then required for the F4E-Radwaste methodology as it is intended to be used with CuV meshes for the latest ITER models.

While the D1SUNED patch supports Direct-1-Step Monte Carlo simulations to calculate shut-down dose rates, only the neutron spectra results are of interest for this methodology. Therefore, the D1SUNED runs on “PROMPT” mode and neutrons are the only type of particle transported in the simulation.

In this step, the model specification is introduced as input; it includes the neutron source, the geometry of the model (including the geometry of the system under study) and the superimposed mesh parameters like its location, coordinates type (cartesian or cylindrical) and discretization both spatial and in energy. The mesh parameters will remain the same for the following steps.

The material compositions are defined also in the input for the simulation. While the material composition of the geometry is defined in this step and will not change for the rest of the methodology, the nuclear data libraries used for the radiation transport could be different to the ones used in the activation calculation, for this reason they appear as a new input in the diagram of Figure 1.

As result of the neutron transport simulation, a file is produced containing the neutron spectra values. There will be an independent value for each combination of:

1. Voxel
2. MCNP cell inside the voxel
3. Energy bin

3.3. Activation calculation

The activation calculation takes as input the neutron spectra produced at the previous step as well as the material compositions and, by solving the Bateman equations, the activity of a set of isotopes is calculated. The activation calculation software employed in this methodology is R2SUNED [R5] which is based on the ACAB code [R13].

R2SUNED is a code that has Rigorous-2-steps capabilities for the calculation of shut-down dose rates. This methodology is concerned only on the radwaste classification of components and therefore it only partially utilizes the R2SUNED code. In a R2S calculation, the neutron spectra data is used to calculate the activation of materials, this activation information is used to generate a gamma source and then the gammas are transported in a secondary Monte Carlos simulation. F4E-Radwaste stops the R2S workflow once the activation data is produced, this activation data is then post-processed in the remaining steps of the methodology.

R2SUNED only computes the activation of a set of isotopes that can be specified by the user. For the purposes of F4E-Radwaste in the ITER context, a thorough list that includes exactly 800 isotopes has been prepared. This list includes all the isotopes that are tracked for the radwaste classification according to the relevant French regulations and many more to cover all the considered relevant contributors to the activity of the

radwaste packages. The isotope list was defined in [R6]. See Appendix B for information on how to modify the isotope list if deemed necessary.

As input of the activation calculation an irradiation scenario is defined including all the decay times of interest. The decay times will not be modifiable in the following steps. Each extra decay time included will increase the volume of the results and therefore selecting many of them in a single activation calculation could hinder the performance of the post-processing and produce errors due to insufficient RAM memory. The size of the results greatly depends on the complexity of the model and the resolution of the mesh. As an example, a calculation for an ITER system in the 360-degree model of the tokamak with a mesh of 66300 voxels can handle a set of 5 different decay times with relative ease in a work laptop with 16 Gb of RAM memory.

The result of this step is a file containing the specific activity in Bq/cc for every combination of:

1. Voxel
2. MCNP cell inside the voxel
3. Decay time
4. Isotope

Note that in the units of Bq/cc, the volume refers to that of the portion of the cell inside the voxel.

3.4. Post-processing

The results of the previous step have units of Bq/cc while the relevant radwaste regulations specify limits and parameters in Bq/g. In the post-processing step of the methodology the activation results are converted to Bq/g, the radwaste classification criteria are applied and the results are formatted in a way that allows its analysis and interpretation.

The results needed for the next step consist in a table with the activity data, a table with the mass data and a file with the mesh parameters. In addition to these results, the post-processing also produces extra data files that are already useful by themselves to analyse the components, even though they are insufficient to determine the radwaste classification of a package. There are three types of post-processing strategies available to the user, the selected strategy will determine the type of post-processing files produced at this step. Independently of the processing strategy, results will include not only the specific activity of every isotope in Bq/g but also all the relevant radwaste parameters like the total activity, IRAS, LMA and mass. Appendix C includes a brief explanation on the way the data is post-processed; when combining several data points of a CuV mesh, it is not possible to simply sum or average the values, hence the need of specific post-processing functions and strategies within the F4E-Radwaste tool.

3.4.1. Standard processing

This processing strategy is the one that requires less input and preparation on the user's side. In addition to generating the data tables with all the information needed for the next step, the processing will generate an extra set of CSV and VTK files. These extra files contain the radwaste relevant information organized in a 3D mesh where every voxel contains results for a specific set of conditions:

1. Material
2. Decay time

The VTK file is a 3D representation of the mesh while the CSV file contains the same information tabulated. There is a pair of CSV/VTK files for each combination of material and decay time present in the model. It is to be expected that in a complex model with many different materials, for any given mesh most of its voxels will be empty, only showing information in the specific locations where the components of the specified material are located. Besides producing a mesh for every material-decay time combination, an extra mesh is produced for each decay time that combines the results of all the materials.

3.4.2. Cell-filtered processing

This processing strategy is analogue to the standard processing applying a filter to the MCNP cells that will be considered. It requires of an extra input file with the set of MCNP cell ids to consider. Any cell not specified in the filtering file will not contribute to the activity nor the mass of the processed results. The resulting files of this strategy are the same as those of the standard process. This strategy can be used to counter the presence of neighbouring components or geometry to the component under study. It can also be used to study a set of components separately from the rest of the model, this is especially useful when some components may be removed earlier than others for maintenance, substitution, or operational requirements during decommission.

3.4.3. By-component processing

This processing strategy will not provide results over a 3D mesh. The processing will collapse the voxel and MCNP cell data into a set of components and provide the results as a table where each row represents a component and the columns carry the radwaste relevant parameters like the specific activity in Bq/g of every isotope, the total activity, the IRAS or the radwaste class. The dose at 1 meter and contact dose rate are also calculated and provided, see Annex D. An input file with the relationship between components and their respective set of MCNP cell ids must be provided. Producing this extra input file is trivial if the F4E nuclear analysis workflow is employed in the preparation of the MCNP input [R1].

This strategy allows the automatic production of ITER radwaste checklists [R14] and provides a straightforward way to analyse the results.

3.5. Package definition and visualization

The data tables generated at the previous step for the standard or cell-filtered options are loaded, visualized and further post-processed. The information loaded consist in a mass table and an isotope activity table. The mass table contains the material and mass information in grams for every combination of:

1. Voxel
2. MCNP cell

The activity table contains the absolute activity values in Bq for every combination of:

1. Voxel
2. MCNP cell
3. Decay time
4. Isotope

The GUI allows the visualization of the information in 3D and the application of several formatting options.

The visual representation of the 3D mesh can display information on the specific activity of any given isotope or radwaste relevant parameters like the IRAS for any combination of material and decay time. The user can also select the option to see the results of the combination of all the materials for a given decay time or create custom material combinations. Every time the user selects a new combination of material and decay time, the GUI will post-process the data tables on the fly to collapse the relevant data into their correspondent voxels.

Geometry files can also be provided for visualization purposes. This way, the user can prepare the CAD equivalent of a combination of materials and then sample over it the radwaste relevant results.

Finally, radwaste packages can be defined via the GUI as a box superimposed to the geometry or by importing a CAD prepared with another software. The radwaste package can be post-processed on-the-fly, collapsing all the data found inside it into a single set of radwaste relevant parameters including the radwaste classification of the package and its mass.

These results are displayed directly on the GUI but can also be printed on a file.

By experimenting and studying the results the user can design and optimize a packaging strategy. Via the modification of size, location and materials included in the package, the amount of mass classified with a specific radwaste level will vary. Usually, the objective of the user will be to minimize the amount of mass classified with the higher radwaste levels. The tool can also be used simply to make predictions on the amount and classification of packages already defined by other constraints.

4. Installation and setup

4.1. Getting the software

There are 3 main pieces of software required for the methodology:

1. MCNP + D1SUNED: neutron transport calculation
2. R2SUNED: activation calculation
3. F4E-Radwaste tool: post-processing, visualization, and packaging

The distribution of MCNP, D1SUNED and R2SUNED is out of the scope of this document. They are proprietary pieces of closed software. F4E-Radwaste tool is a FOSS (Free and Open-Source Software) which can be obtained by requesting it to the F4E nuclear team or directly by downloading it from its GitHub page [R15].

4.2. Installing the software

4.2.1. Installation of MCNP5 and D1SUNED

The installation of MCNP and the application of the D1SUNED patch are out of the scope of this document.

4.2.2. Installation of R2SUNED

Due to the proprietary nature of the R2SUNED code, it cannot be distributed along the F4E-Radwaste tool that can be found on GitHub. To install the R2SUNED code, it is assumed that the user has received a folder called **R2SUNEDV2** with the contents seen in Figure 2.

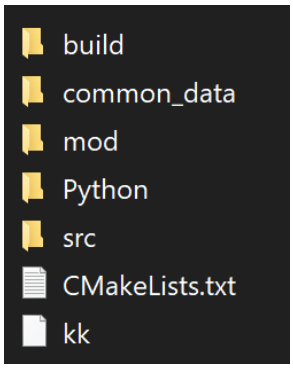


Figure 2 - Contents of the R2SUNEDV2 folder

The steps to perform the installation are as follows:

1. Copy the R2SUNEDV2 folder on the desired location of the machine where this code will run. The machine should run under a Linux distribution.
2. Remove everything inside the **build** folder if it is not already empty.
3. Enter the **build** folder via the command prompt.
4. Load the **cmake** and **Intel** modules by running this set of commands:

   >>>module add
   >>>module add intel/pe-xe-2018--binary
   >>>module add intelmpi/2018--binary
   >>>module add cmake/3.18.2
5. Run the **cmake** command:

   >>>cmake ../
6. Compile via the make command:

   >>>make
7. [Optional] Remove the unnecessary ***mod** files via the command:

   >>>rm -r -f *mod

The installation of the R2SUNED code is now complete. The executable **r2sunedv2.exe** should have been created.

R2SUNED will make calls to some python scripts at the beginning of its execution. For that reason, a folder with the contents seen in Figure 3 must be placed in a location accessible by the R2SUNED code. This folder and a Python script called **preR2SUNED.py** should be provided along with the R2SUNED distribution. It is necessary to modify the contents of the **preR2SUNED.py** file to update the paths to the folders of Figure 3.

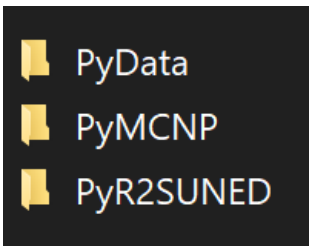


Figure 3 – Contents of the PythonModules folder

The installation of Python on the Linux machine where R2SUNED is installed is out of the scope of this document.

4.2.3. F4E-Radwaste tool

Once the user has downloaded the code from GitHub or received by other means from F4E, the folder containing the code should be placed in a location within a Windows machine with an environment of Python 3.11 installed. Installing and managing Python environments is out of the scope of this document.

To install the tool, the user should enter the code folder via the terminal of the Python environment. Inside the folder, and among other files and folders there should be a file called **setup.py**. Run the command:

>>>pip install .

All the necessary dependencies will be installed automatically and the F4E-Radwaste tool will be added to the list of installed modules of the Python environment. To start the program and its GUI the user can run the command:

>>>python -m f4e_radwaste

5. Operation

This section explains all the steps and files required to perform an analysis with the F4E-Radwaste methodology. Figure 4 presents a flow diagram showing the most important files involved in the methodology.

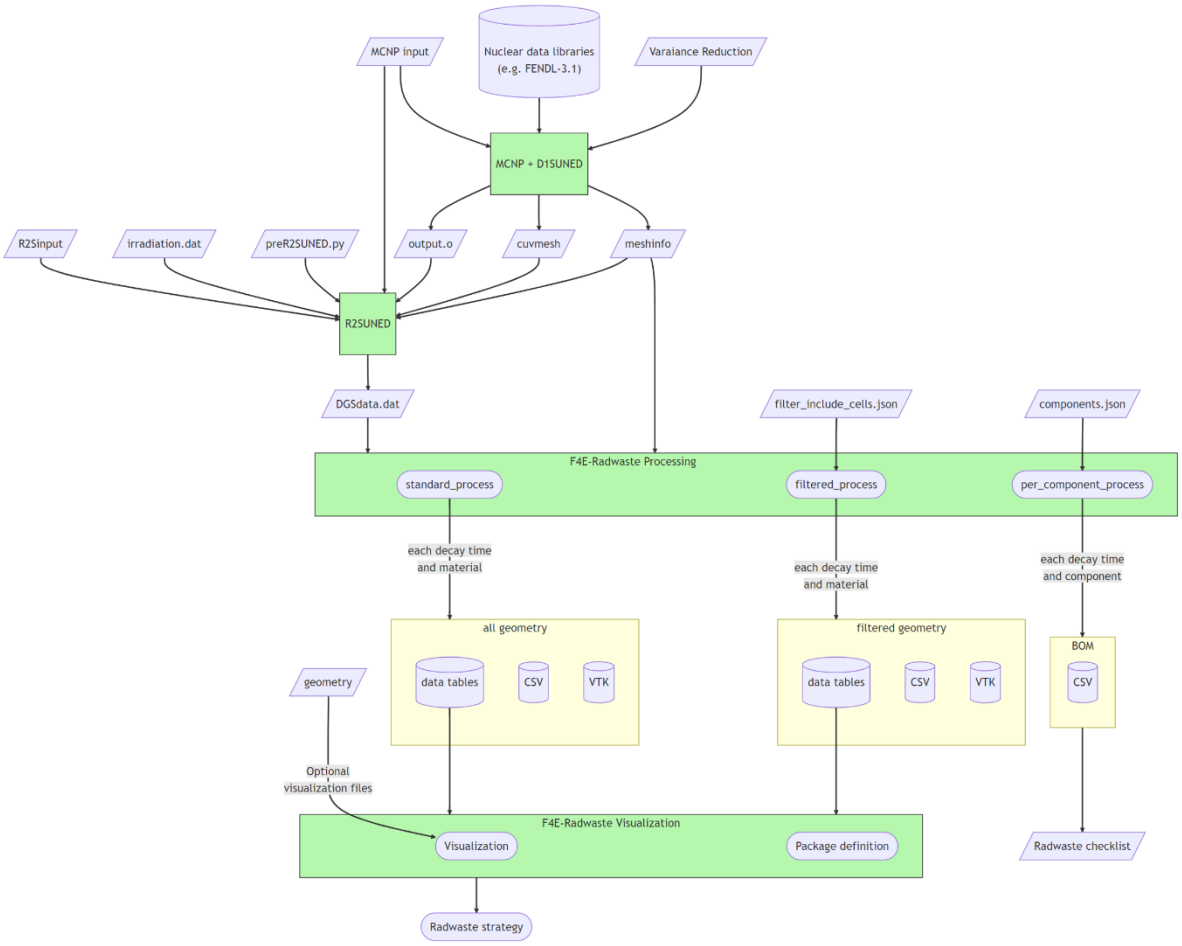


Figure 4 - Overview of the files and data flow

5.1. Neutron transport

The neutron transport calculation is done through MCNP5 + D1SUNED3.1.4. The specific considerations to perform the Monte Carlo simulation for the F4E-Radwaste methodology are presented in this section. A general explanation of how to prepare and run an MCNP simulation and the theory behind it are out of the scope of this document.

The main input file in this step is the MCNP input (which is also required as input in the activation calculation). Optionally, a file dedicated to the variance reduction may be employed too. In the MCNP input file are defined the model geometry, the material compositions, the particle source, and the parameters of the mesh superimposed to the geometry of study.

The input file should run in neutron only mode as the only parameter of interest is the neutron spectra over the superimposed mesh. To select the neutron mode the input file shall include the **MODE N** card.

The input file should include the **PRMPT** card to avoid that the simulation run in the D1S. While this should not have any noticeable effect as only neutrons are being transported and recorded, it is a good practice to avoid confusion.

The particle source should be a neutron source whose particles start with a statistical weight of 1.

The nuclear data libraries to be used for the transport and the material compositions are also defined in the MCNP input file.

The mesh superimposed to the geometry that will be used for the rest of the methodology is defined in this step as a **FMESH** card. The mesh should cover all the geometry of interest. The resolution of the mesh should be appropriate for the level of detail desired considering the computer resources available. Avoid extending

the mesh much further away from the geometry of interest to reduce the size of the resulting files and further processing times.

```
fmesh4:n geom=cyl
         axs = 0 0 1
         vec = 1 0 0
         origin 0 0 0
         imesh  100             iints 30
         jmesh  550             jints 50
         kmesh  1               kints 36
         emesh
         1.00001e-07  4.13994e-07  5.31578e-07  6.82560e-07  8.76425e-07
         1.12535e-06  1.44498e-06  1.85539e-06  2.38237e-06  3.05902e-06
         3.92786e-06  5.04348e-06  6.47595e-06  8.31529e-06  1.06770e-05
         1.37096e-05  1.76035e-05  2.26033e-05  2.90232e-05  3.72665e-05
         4.78512e-05  6.14421e-05  7.88932e-05  1.01301e-04  1.30073e-04
         1.67017e-04  2.14454e-04  2.75364e-04  3.53575e-04  4.53999e-04
         5.82947e-04  7.48518e-04  9.61116e-04  1.23410e-03  1.58461e-03
         2.03468e-03  2.24867e-03  2.48517e-03  2.61259e-03  2.74654e-03
         3.03539e-03  3.35463e-03  3.70744e-03  4.30742e-03  5.53084e-03
         7.10174e-03  9.11882e-03  1.05946e-02  1.17088e-02  1.50344e-02
         1.93045e-02  2.18749e-02  2.35786e-02  2.41755e-02  2.47875e-02
         2.60584e-02  2.70001e-02  2.85011e-02  3.18278e-02  3.43067e-02
         4.08677e-02  4.63092e-02  5.24752e-02  5.65622e-02  6.73794e-02
         7.19981e-02  7.94987e-02  8.25034e-02  8.65169e-02  9.80366e-02
         1.11090e-01  1.16786e-01  1.22773e-01  1.29068e-01  1.35686e-01
         1.42642e-01  1.49956e-01  1.57644e-01  1.65727e-01  1.74224e-01
         1.83156e-01  1.92547e-01  2.02419e-01  2.12797e-01  2.23708e-01
         2.35177e-01  2.47235e-01  2.73237e-01  2.87247e-01  2.94518e-01
         2.97211e-01  2.98491e-01  3.01974e-01  3.33733e-01  3.68832e-01
         3.87742e-01  4.07622e-01  4.50492e-01  4.97871e-01  5.23397e-01
         5.50232e-01  5.78444e-01  6.08101e-01  6.39279e-01  6.72055e-01
         7.06512e-01  7.42736e-01  7.80817e-01  8.20850e-01  8.62936e-01
         9.07180e-01  9.61640e-01  1.00259e+00  1.10803e+00  1.16484e+00
         1.22456e+00  1.28735e+00  1.35335e+00  1.42274e+00  1.49569e+00
         1.57237e+00  1.65299e+00  1.73774e+00  1.82684e+00  1.92050e+00
         2.01897e+00  2.12248e+00  2.23130e+00  2.30686e+00  2.34570e+00
         2.36525e+00  2.38521e+00  2.46597e+00  2.59240e+00  2.72532e+00
         2.86505e+00  3.01194e+00  3.16637e+00  3.32871e+00  3.67879e+00
         4.06570e+00  4.49329e+00  4.72367e+00  4.96585e+00  5.22046e+00
         5.48812e+00  5.76950e+00  6.06531e+00  6.37628e+00  6.59238e+00
         6.70320e+00  7.04688e+00  7.40818e+00  7.78801e+00  8.18731e+00
         8.60708e+00  9.04837e+00  9.51229e+00  1.00000e+01  1.05127e+01
         1.10517e+01  1.16183e+01  1.22140e+01  1.25232e+01  1.28400e+01
         1.34986e+01  1.38403e+01  1.41907e+01  1.45499e+01  1.49183e+01
         1.56831e+01  1.64872e+01  1.69046e+01  1.73325e+01  1.96403e+01
         out=cuv
         sppts= 1000 spmode=rand
```

Figure 5 - FMESH example

The mesh can be defined with cartesian or cylindrical coordinates. Keep in mind that cylindrical coordinates have voxels that vary their volume radially and that plotting and working with them is slightly more inconvenient than with cartesian coordinates. It is recommended to choose cartesian coordinates unless the use of cylindrical is especially convenient due to the geometry of interest. The energy discretization of the results is defined as a mesh parameter by means of an **emesh** card. Although any discretisation format available in the activation libraries can be used, the Vitamin J format is recommended: it consists in 175 energy bins that range between 1e-7 to 19.6403 MeV.

The mesh must be defined as a CuV tally by means of including the **out=cuv** card. Refer to the D1SUNED manual for a more detailed explanation [R3]. When using a CuV mesh, the radiation transport code needs to calculate the proportion of volume occupied by every cell inside a given voxel. This is done by sampling a set of points inside the voxels and determining in which MCNP cell they are contained. The quality of this sampling will determine the accuracy of the partial volume results. The sampling strategy is specified by including the card **sppts=-1000 spmode=rand**, where -1000 indicates a sampling density of 1000 points per cubic centimetre and rand a uniform random sampling for the location of the sampling points. The mesh should not have any normalization or multiplication card applied. See Figure 5 for an example of the FMESH definition with cylindrical coordinates and a Vitamin J energy discretization.

As with any other MCNP simulation, the use of variance reduction techniques like particle splitting and Russian roulette via a GVR are allowed and can be very beneficial regarding the statistical uncertainty of the results.

The neutron transport simulation will produce 3 files that are required for the following steps of the methodology: the cuvmesh file, the meshinfo file and the MCNP output file.

5.2. Activation calculation

The activation calculation is performed with the R2SUNED code, and it requires many input files and preparation. The simplest way to prepare the simulation is to put all the required files in a folder that contains the **r2sunedV2.exe**, this executable can be copied and pasted in any folder. The files required for any specific calculation are:

1. inputR2S [Filename can't be modified]
2. cuvmesh
3. meshinfo
4. MCNP output
5. MCNP input
6. irradiation_scenario.dat [Filename can't be modified]
7. preR2SUNED.py [Filename can't be modified]
8. PHOTON.dat [Filename can't be modified]

5.2.1. inputR2S

The **inputR2S** file should be found in the same folder as the **r2sunedV2.exe**, the name of the file must remain "inputR2S" without any file suffix. This file contains the main activation parameters and paths to the other input files. There are many parameters and input options in this file that are not relevant for the F4E-Radwaste methodology and some others, while relevant, do not need to be changed by the user. The input options that the user needs to consider when modifying the inputR2S template file are presented in this section.

At the beginning of the file there is a set of variables to be filled with the location of the folders and files of interest. The ones the user needs to consider are:

1. data_path. Path to the **common_data** folder, which is included in the R2SUNED distribution, see Figure 2.
2. cuvmsh_path. Path to the cuvmesh file produced at the radiation transport calculation.
3. meshinfo_path. Path to the meshinfo file produced at the radiation transport calculation.
4. outp_path. Path to the MCNP output file produced at the radiation transport calculation.
5. mcnp_input. Path to the MCNP input file used during the radiation transport calculation.

The rest of the path files are not relevant for the activation calculation.

Below the path files section there are other options that the user is not required to modify until the area regarding the decay times. The **ntime** and **TimeDGS** keywords indicate the amount of different decay times that are requested in the calculation, both should be filled with the same amount. Below them, each decay time is defined. The keyword **last** indicates that the specified time is related to the time passed since the end of the last irradiation phase. The irradiation_scenario.dat should include in its phase after the last irradiation a time at least as big as those required in the activation calculation, see Appendix A for a detailed explanation.

```
ntime= 5
TimeDGS    5
1y      last  # (s= second, d=day,y=year)
2y      last
5y      last
10y     last
20y     last
```

Figure 6 – Example of decay times definition in the R2SUNED input file

The last parameter that the user may want to modify is the **Filter**. This parameter defines the range of MCNP cell ids that the activation calculation will consider. Currently is set as **1:9999999** to avoid filtering out any cell. It is recommended to not modify this parameter as the cell filtering can be done later in the methodology, in the post-processing step.

5.2.2. cuvmesh file

The file produced by MCNP with the neutron spectra results. It can have a different name and be in another folder if its path is properly accounted for in the inputR2S.

5.2.3. meshinfo file

The file produced by MCNP with the information on the CuV mesh. It can have a different name and be in another folder if its path is properly accounted for in the inputR2S.

5.2.4. MCNP output file

The output file produced by MCNP. In the case the MCNP simulation had to be continued, more than one output file would be produced. The output file required by R2SUNED is the first one, which contains the **Table 60** with the material densities of the cells. It can have a custom name and be in another folder if its path is properly accounted for in the inputR2S.

5.2.5. MCNP input file

The input file used by MCNP during the neutron transport calculation. It is used to obtain the material composition of the cells. It can have a custom name and be in another folder if its path is properly accounted for in the inputR2S.

5.2.6. preR2SUNED.py

The **preR2SUNED.py** file should be found in the same folder as the **r2sunedV2.exe**, the name of the file must remain “preR2SUNED.py”. The paths specified in this file should correctly point to the folders of Figure 3.

5.2.7. irradiation_scenario.dat

The **irradiation_scenario.dat** file should be found in the same folder as the **r2sunedV2.exe**, the name of the file must remain “irradiation_scenario.dat”. Contains the irradiation phases and decay times to be considered in the activation calculation in a specific format. See Annex A for an explanation on how to modify this file to account for custom irradiation scenarios.

5.2.8. PHOTON.dat

The **PHOTON.dat** file should be found in the **common_data** folder inside **R2SUNEDV2** as seen in Figure 2, the name of the file must remain “PHOTON.dat”. This file contains a list of the isotopes whose activity will be tracked in the activation calculation. That is, only the isotopes present in this file will be able to appear as a result. It is recommended to keep the extensive 800 isotopes list defined in [R6] as a shorter list may miss some relevant isotope. See Appendix B for an explanation on how to modify this file.

The result of the activation calculation is a single file called **DGSdata.dat**.

5.3. Post-processing

This step is performed with the F4E-Radwaste tool which is operated via a GUI. Via the

>>>python -m f4e_radwaste

command, the GUI will be opened in a new window as seen in Figure 7. The user will operate the program via the GUI while some information regarding the state of the processing will be displayed in the terminal that was used to launch the GUI. To run the post-processing functions, open the **Processing** menu at the top left corner and select one of the 3 processing strategies, see Figure 8. A new window will be opened to allow the user to browse the machine files and select the folder containing the necessary input files. After the processing is done, a new folder named **results** will appear at the same location of the input files. This folder will contain the processed files.

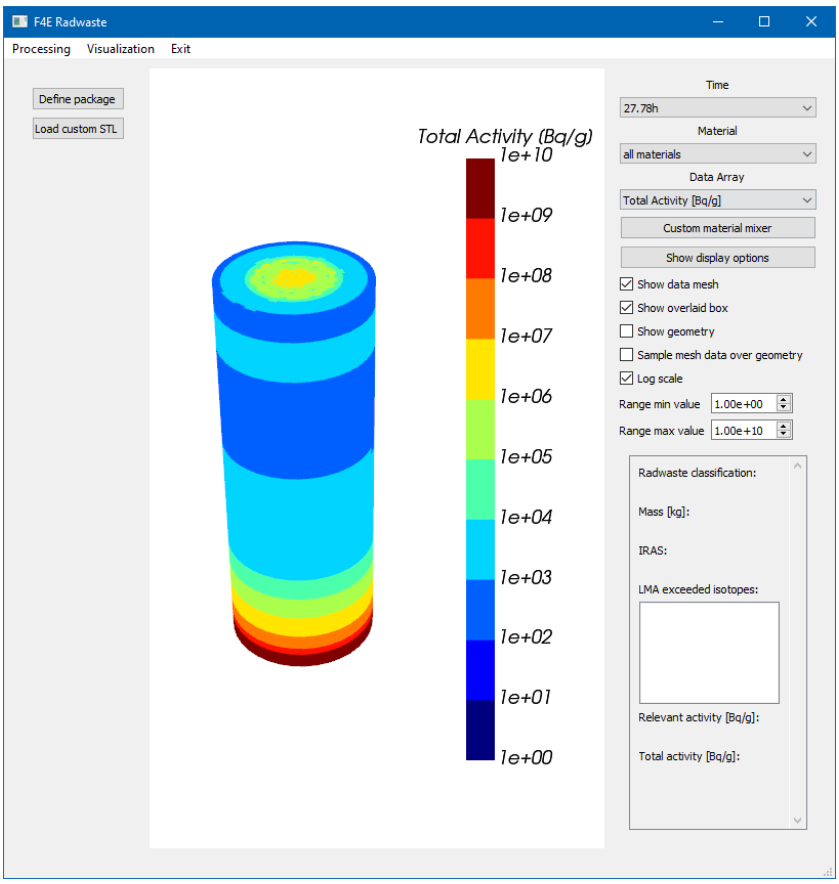


Figure 7 - F4E-Radwate tool GUI overview

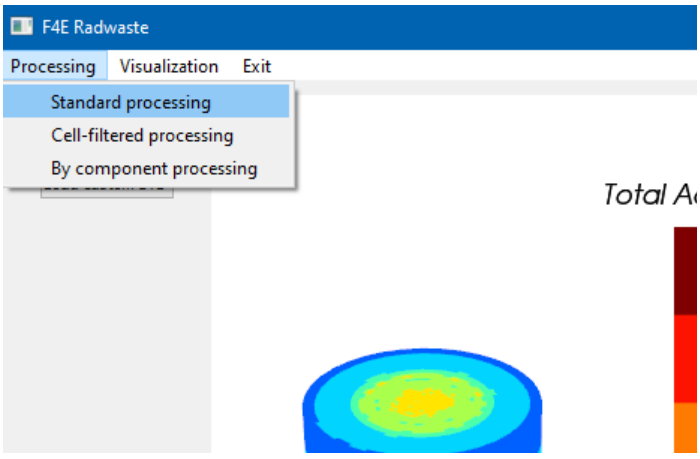


Figure 8 - Detail of the Processing menu

5.3.1. Standard processing

The inputs required for the standard processing are the **DGSdata.dat** file and the **meshinfo** file. Both files should be present in the folder selected by the user, the filenames should not be modified. The tool will automatically read the files and perform the data processing. This operation may take from a few seconds to a few minutes. Messages updating the state of the process will be displayed in the terminal. In the **results/data_tables** folder, the required inputs for the visualization and package definition step are stored. The mesh data VTK and CSV files generated for each combination of decay time and material are stored in **results/vtk_files** and **results/csv_files** respectively. These files can already be of use to do a preliminary assessment of the radwaste relevant parameters that the geometry of interest is subjected to.

5.3.2. Cell-filtered processing

The cell-filtered processing is analogue to the standard one, but it requires an extra file, the **filter_include_cells.json**. This file is a JSON file with the format as seen in Figure 9. The cell ids that form the list “cells_to_include” will be the only ones that will be considered in the post-processing which will prepare the resulting data tables as well as the CSV and VTK files with the data collapsed in every combination of material and decay time.

```
{"cells_to_include": [940000, 940001,
                      940003, 942068]}
```

Figure 9 - filter_include_cells.json example

5.3.3. By component processing

This processing strategy is different to the standard and filtered ones in the sense that its only output is a set of CSV files, it will not produce the data tables required for the package definition and visualization, nor the VTK files. Instead, it produces a set of CSV files (one per decay time) where each row represents a component.

This functionality requires two extra input besides the **DGSdata.dat** and **meshinfo** files, the **components.json** and the **auxUMdata.inp**. The **components.json** file is a JSON file with the format of Figure 10. It consists in a list of lists (each member representing a component). Each component starts with a string with the component’s name and then, as a second item, a list with the MCNP cell ids that form the component.

```
[
    ["RESIDENT_GUIDE_END_STOP_BLOCK#LXXQ6B", [940000]],
    ["RESIDENT_GUIDE_REAR_DISC_SPRING#LXXQGE", [940011]],
    [
        "IVV_PSE_ELECTRICAL_HEATER_LH#WAP3NS",
        [
            942055,
            942056,
            942057,
            942058,
            942059,
            942060,
            942066
        ]
    ],
    ["HEATING_JACKET_FOR_IVV_PE_AT_PORT#XCCZ5G", [942068]]
]
```

Figure 10 - components.json example

The **auxUMdata.inp** is a file that is automatically generated by R2SUNED during the activation calculation. The user may make a copy of it and place it with the other post-processing input files. This file contains the isotope distribution of every material, necessary for the calculation of the contact dose rate factors.

The resulting CSV will provide radwaste relevant parameters including mass and radwaste class of each component defined in the JSON file as well as the dose at 1 meter and contact dose rate. This information is especially useful to prepare a radwaste checklist. In a radwaste checklist the specific activities of certain isotopes are required for the list of components that forms a system. See Figure 11 for an example of the results.

	A	B	C	D	E	F	G	H	I	J	K
1	Voxel	Dose 1 meter [Sv/h/g]	Contact dose rate [Sv/h]	Radwaste class	IRAS	LMA	Total Activity [Bq/g]	F	Mass [g]	C14	Co58
17	RESIDENT_GUIDE_CAPTIVE_TRACK_RH#LXXQEF	2.66E-10	1.55E-04	Type A	2.09E+01	0.00E+00	5.95E+02		4.36E+04	3.23E-02	5.25E-01
18	RESIDENT_GUIDE_CAPTIVE_TRACK#LXXQCG	2.67E-10	1.55E-04	Type A	2.10E+01	0.00E+00	5.46E+02		4.42E+04	2.72E-02	7.67E-01
19	RESIDENT_GUIDE_CARTRIDGE_V_RAIL#LXXQ8A	2.46E-10	1.43E-04	Type A	1.92E+01	0.00E+00	5.02E+02		1.09E+04	3.78E-02	5.15E-01
20	RESIDENT_GUIDE_CARTRIDGE_V_RAIL#LXXQ8A	2.40E-10	1.39E-04	Type A	1.86E+01	0.00E+00	5.45E+02		1.09E+04	4.55E-02	2.73E-01
21	IVVS_PORT_FIXATION#SMCGA3	9.07E-11	5.28E-05	Type A	7.03E+00	0.00E+00	1.68E+02		2.04E+04	7.59E-03	1.03E-01
22	CR_LC_IVV_SUPPORT_SHIM_PLATE#VRGNRM	8.52E-11	4.95E-05	Type A	6.57E+00	0.00E+00	1.49E+02		1.01E+04	6.38E-03	8.98E-02
23	IVVS_ARM_CHASSIS#LXXQZN	4.57E-10	2.63E-04	Type A	3.81E+01	0.00E+00	9.48E+02		6.32E+03	3.69E-02	6.80E+00
24	IVVS_ARM_HINGE#LXXR3M	4.27E-10	2.47E-04	Type A	3.48E+01	0.00E+00	8.39E+02		2.03E+03	3.43E-02	5.10E+00
25	IVVS_ARM_CAPTIVE_SCREW_M10#LXXR9J	2.29E-10	1.28E-04	Type A	2.03E+01	0.00E+00	7.37E+02		2.95E+01	3.46E-02	9.29E+00
26	IVVS_ARM_CAPTIVE_SCREW_M10#LXXR9J	1.65E-10	9.61E-05	Type A	1.29E+01	0.00E+00	3.62E+02		2.90E+01	1.82E-02	1.11E-01
27	IVVS_TROLLEY_BOTTOM_HINGE_PIN#LXXVFQ	9.19E-13	4.31E-07	TFA	4.42E-01	0.00E+00	3.17E+02		3.68E+01	8.72E-02	5.38E-01
28	IVVS_TROLLEY_CHASSIS#26Y9XT	2.50E-10	1.45E-04	Type A	1.96E+01	0.00E+00	5.25E+02		6.38E+04	2.67E-02	8.75E-01
29	KOYO_BEARING_80OD_40ID_18W#LXXUJ2	1.33E-10	7.73E-05	Type A	1.02E+01	0.00E+00	2.35E+02		5.18E+02	1.04E-02	1.76E-06

Figure 11 - CSV example result of a by component processing

5.4. Package definition and visualization

To start the visualization and package definition process, the first step is the loading of the data tables produced at the post-processing step via the standard or cell-filtered processing. To load the data tables, click on the Visualization menu found in the top left corner of the F4E-Radwaste window and select then click on the unfolded button. This will open a new window that the user will use to navigate through the folders of the machine and select the **data_tables** folder generated in the processing step.

The files will be immediately loaded into the program and the resulting mesh will be displayed on the screen. Depending on the size of the files, the loading may take up to a few seconds. In the right side of the screen there are several visualization options, see Figure 12. The **Time**, **Material** and **Data Array** selection wheels selection of the displayed mesh. Via **Time** and **Material**, the decay time and material/s to display are selected. Every time a decay time or a material is changed, the F4E-Radwaste tool will perform a post-processing calculation to collapse the relevant data from the data tables into the displayed mesh. If the size of the data tables is significant this operation could take 1 or 2 seconds to perform. At the bottom of the **Material** selection list there are two special options: **all materials** and **custom material**. The **all materials** option will output results that are a combination of all the materials present in the data tables. The **custom material** option allows the display and manipulation of an arbitrary combination of materials. Before selecting, the user should click on the button **Custom material mixer**. This will open a new window with the list of materials present in the data tables, the user may select from the list all the materials needed for the combination and then close the window. After that, selecting the **custom material** option in the **Material** wheel will perform the material combination processing and display the results.

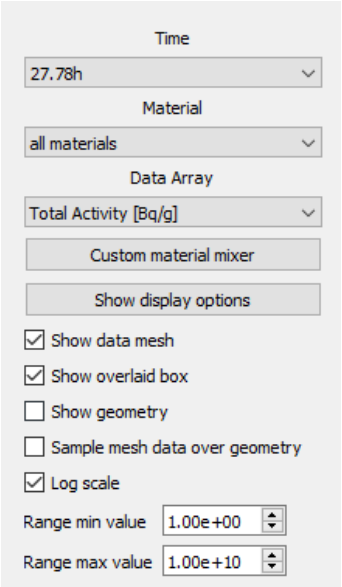


Figure 12 - Data selection and visualization options

The **Data Array** wheel allows the selection of the radwaste relevant parameter to display in the mesh. Changing the data array will not trigger the post-processing of the data tables and therefore this operation

should be almost immediate even for the biggest meshes. Among the possible list of data arrays there are the specific activities of every relevant isotope in Bq/g, the IRAS parameter, the number of LMA exceeded isotopes, the radwaste class and the mass of the selected materials inside the voxels. The user can tick the tick box **Log scale** to switch on and off the logarithmic scale of the data array colour range. Below the **Log scale** box, there are two input wheels showing the lower and upper values of the range, the user can manually modify those values.

There are 2 ways to define a radwaste package:

1. Use the GUI to generate a superimposed box by defining its size, and location.
2. Import a CAD geometry defined in other software.

To generate the package via the GUI, click the **Define Package** button found at the left of the screen. A parallelepiped that fits the whole displayed mesh will be generated immediately. If the **Show overlaid box** tick box found on the right of the window is selected, the package geometry will be visible. Unselect the tick box to hide the package geometry, this will not delete or modified the actual package. Notice that the button layout at the left of the screen has changed. The user can modify the **Origin**, **Size** and **Rotation** wheels to manipulate the package geometry, see the detail of Figure 13, these wheels are found on the left side of the screen.

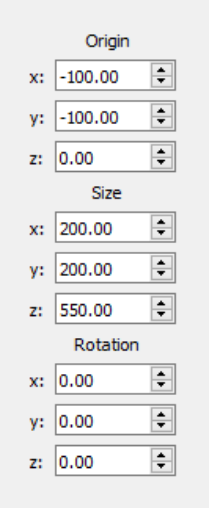


Figure 13 - Package 3D parameters

To import a CAD geometry as the package, click the **Load Custom STL** button instead of the **Define Package** one. When importing the package geometry, a new window will be opened to browse through the directories of the machine. The file format of the package geometry should be STL. Notice that the layout on the left side of the screen also changes after the import.

After generating or importing the package geometry here are three new buttons on the left side of the screen. The **Delete Box** button will delete the package geometry which in turn allows importing or generating a new one.

The **Calculate radwaste** button will calculate the radwaste relevant parameters found inside the package for the selected decay time and material combination. The most relevant radwaste results of the package will be then updated in the sub-window found at the bottom right corner of the main window. Depending on the size of the mesh and its data, this processing step could take up to 1 or 2 seconds.

The **Print radwaste info** button will output all the calculated radwaste parameters inside the package to a file called **PACKAGE.csv**. This file is in CSV format and will be saved into the same folder where of the data tables used to load the mesh. If many different packages are to be exported the recommended approach is to change the name of the files to a custom one every time one is generated.

6. Advanced features

6.1. Plotting the geometry of the components

It is possible to plot the geometry of the components in the GUI alongside the data mesh visualization. For that matter, the user should prepare in another software the CAD files.

The recommended format of the CAD files is PLY, STL will also work but it is less performant. All the CAD files should be placed in a folder called **geometry** which has to be located inside the **data_tables** folder that was used to load the post-processed activity data. The names of the CAD files should be those of the MCNP material ids found in the MCNP model geometry. For example, the file **940001.ply** would contain the CAD geometry related to the material M940001 in the MCNP model.

To activate the geometry visualization, tick the **Show geometry** tick box on the right side of the window. If the box is ticked, when selecting a material on the **Material** wheel, the GUI will attempt to load the geometry of that material. If a **geometry** folder is found and, within that folder, a file with the same name as the material is found (the suffix doesn't count) then that CAD file will be loaded. Note that this naming convention also apply to the special names: **all materials** and **custom material**. The user can prepare a file called "all materials.ply" or "all materials.stl" to show a specific CAD when the option to display all the material information at once is selected. The same procedure happens with the custom material option. Clearing the **Show data mesh** tick box will hide the data mesh showing only the CAD geometry. Ticking the **Sample mesh over geometry** tick box would then display the selected data array over the CAD geometry. Note that the resolution of the PLY or STL file will directly impact the resolution of the sampled mesh. If the CAD geometry is not divided into enough facets, the sampling of data should be avoided. See Figure 14 for an example of the window showing CAD geometry, no data sampling applied.

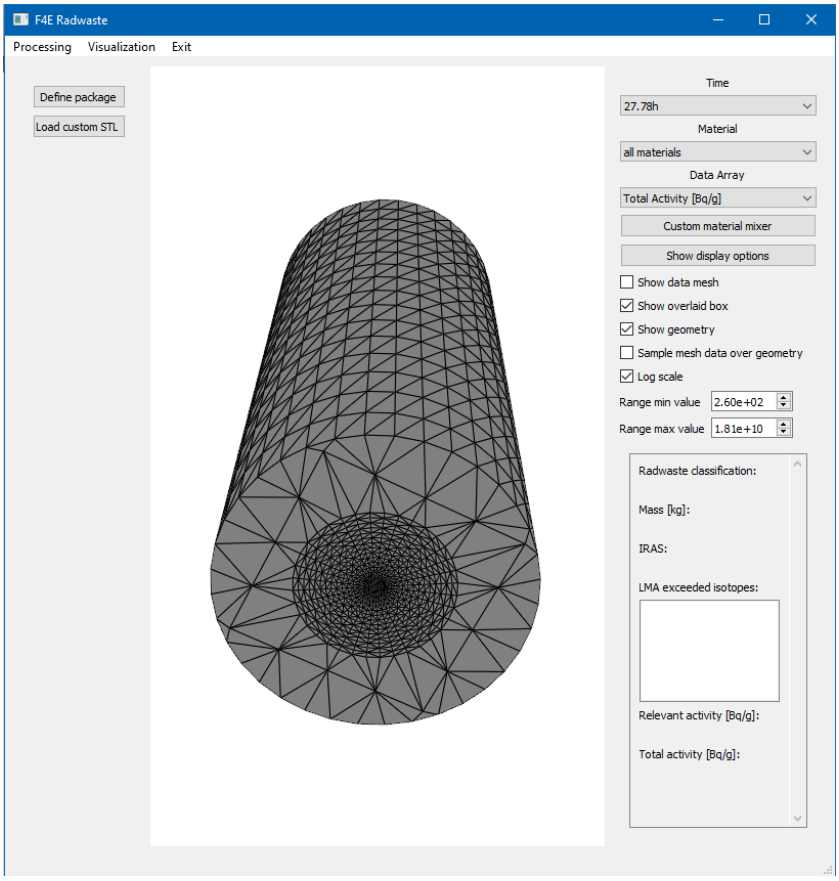


Figure 14 - Geometry files loaded in the GUI

7. ITER 1D benchmark

This section presents an example application of the F4E-Radwaste methodology, the ITER 1D benchmark, a very simple MCNP model that represents the ITER machine.

7.1. Model description

The MCNP model consists of two material cells, each with its own material composition. The plasma source is located at the bottom of Figure 15 pointing upwards. The cylindrical orifice allows the streaming of neutrons and therefore the nuclear responses at the top of the model are a combination deep penetration transport and streaming.

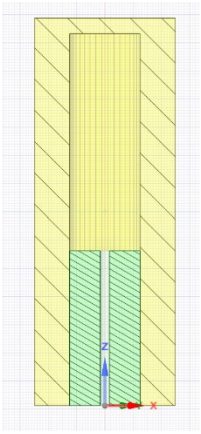


Figure 15 - Scheme of the MCNP model

The whole methodology was applied to the ITER 1D benchmark 2 times, only changing the mesh superimposed to the geometry over which the results were recorded. Both meshes had the same energy discretization, the Vitamin J 175 energy groups.

7.2. Application via cartesian coordinates

The cartesian mesh is a parallelepiped that completely covers all the MCNP geometry. Its voxels consist of cubes of 5cm sides. The total amount of voxels in the mesh is 214896, see Figure 16 for an image of grid.

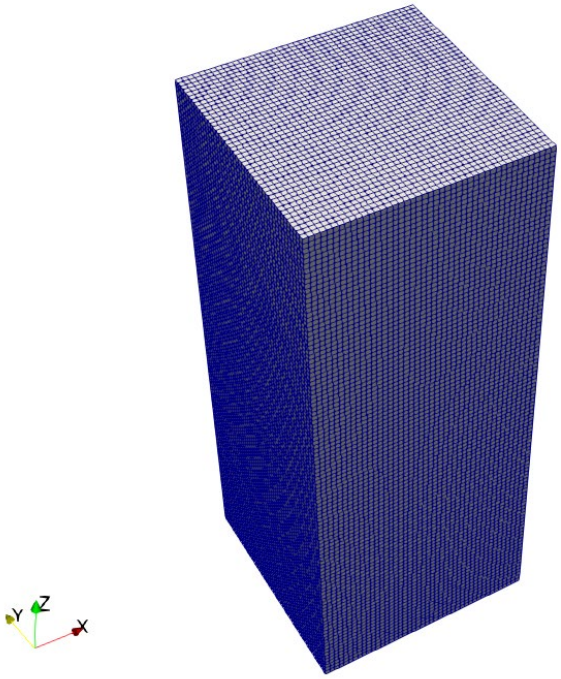


Figure 16 - 3D representation of the cartesian grid resolution

The neutron transport simulation was performed in under 2 hours with 159 cores running in parallel. No variance reduction technique was employed and the total relative error of all the voxels remained below 0.1.

The activation simulation was also performed in less than 2 hours, it employed 46 cores. The post-processing with the F4E-Radwaste tool was performed in a Windows laptop employing a single core, it was finished in under 10 minutes.

7.3. Application via cylindrical coordinates

The cylindrical mesh was lighter than the cartesian mesh, it amounted to 54000 voxels, see Figure 17 for a visual representation. The neutron transport simulation was not significantly affected by the superimposed mesh parameters, they do not affect the particle transport. Therefore, the simulation was performed also in under 2 hours with 159 cores running in parallel. The statistical error of the voxels remained below 0.1. The activation simulation was indeed affected by the smaller size of the results, it was finished in less than 30 minutes with 46 parallel cores. The post-processing of the results with the F4E-Radwaste tool was performed in a Windows laptop employing a single core and it finished in 3 minutes of computation.

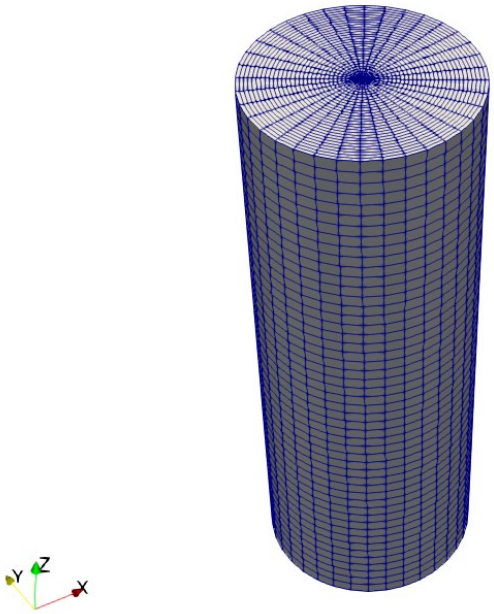
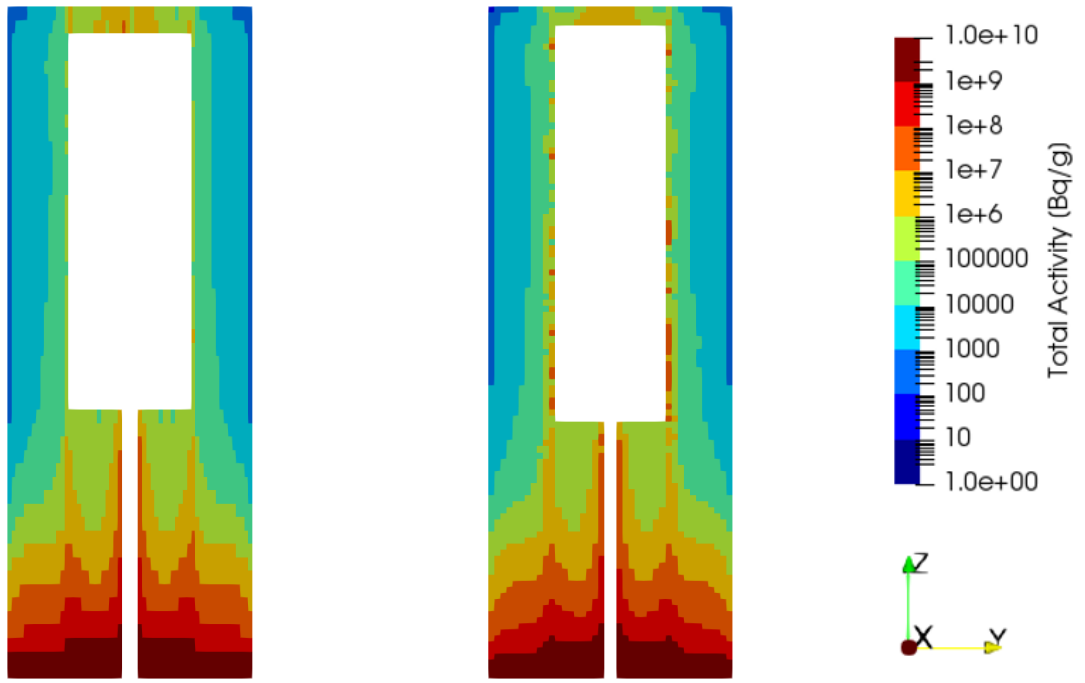


Figure 17 - 3D representation of the cylindrical grid resolution

7.4. Findings

Results were produced for the two types of coordinates. However, the coordinate type should have no significant effect on the analysis. Figure 18 compares the specific activity of the combination of all isotopes between coordinate types. As expected, there are some differences in the visualization due to the different proportion of mass inside the voxels which changes depending on the mesh parameters and coordinate types. The statistical nature of the Monte Carlo method also introduces a degree of variability in the results. The clearest discrepancies are found at the borders of material with void. For the cartesian coordinates, the hollow inside of the cylinders seems smaller due to a bigger proportion of void against the material in the voxels at the border between the two.



(a) Cylindrical coordinates (b) Cartesian coordinates

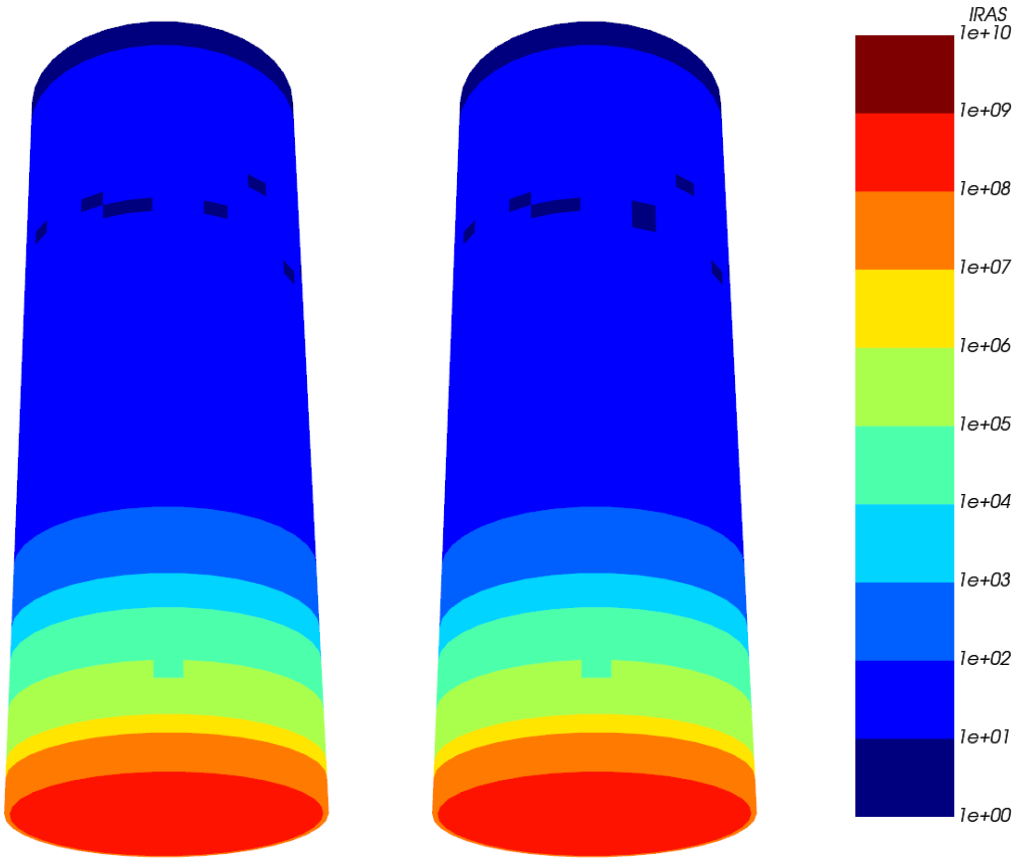
Figure 18 – X-slice comparison of mesh coordinates

Despite the expected small differences due to the mesh parameters and statistic uncertainty, the results look consistent with each other. The rest of the analysis is done via cylindrical coordinates only, reducing redundancy for clarity purposes.

Two decay times were calculated:

1. 1e5 seconds (27.78 hours)
2. 1e6 seconds (11.57 days)

The IRAS values of the voxels at both decay times are represented is a logarithmic scale in Figure 19. There is not a significative difference in the IRAS values due to the short time difference between them. Therefore, it is expected that the radwaste class will not vary between them.



(a) 1e5 seconds (b) 1e6 seconds

Figure 19 - IRAS values depending on decay time

Placing all the geometry of the model in the same radwaste package gives the results seen in Figure 20. The combination of both materials has a weight of 113 tons. The package is classified as Type A for both decay time as their IRAS values is higher than 1. There is no isotope that exceeds its LMA limit.

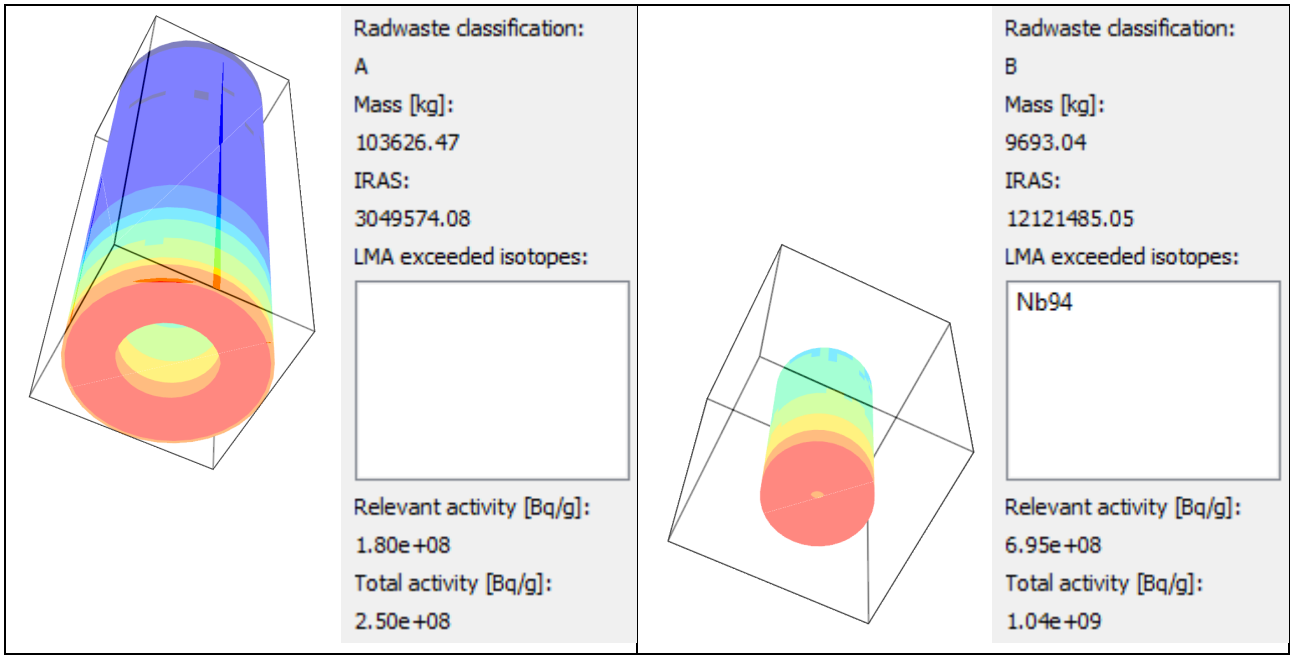
Radwaste classification:	Radwaste classification:
A	A
Mass [kg]:	Mass [kg]:
113319.51	113319.51
IRAS:	IRAS:
3902725.77	3825560.49
LMA exceeded isotopes:	LMA exceeded isotopes:
Relevant activity [Bq/g]:	Relevant activity [Bq/g]:
2.27e+08	2.24e+08
Total activity [Bq/g]:	Total activity [Bq/g]:
3.57e+08	3.17e+08

(a) 1e5 seconds (b) 1e6 seconds

Figure 20 - Package radwaste parameters depending on decay time for all the geometry

Using the material wheel, each of both materials present in the model are selected. The radwaste parameters of a package containing each of the materials at 1e6s of decay time are shown in Figure 21. Material 2 is classified as Type B, higher than Material 1, as the isotope Nb94 exceeds its LMA limit. The main reasons for a higher classification for Material 2 to consider are:

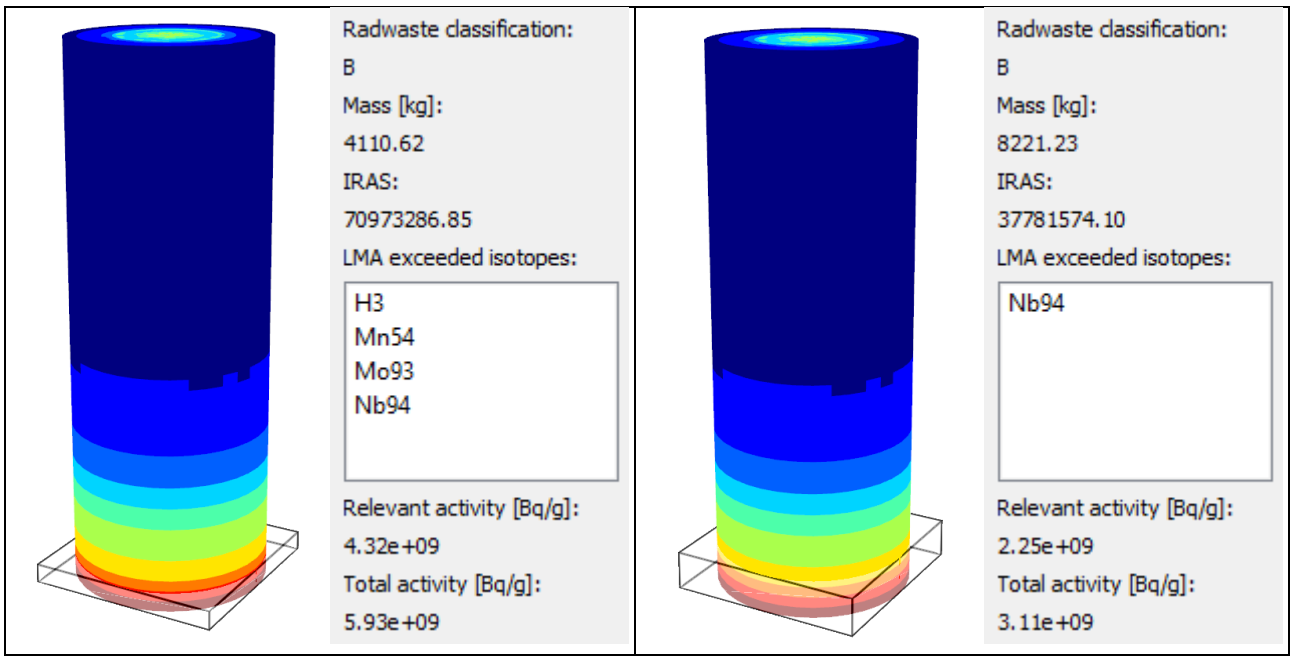
1. The centre of mass is closer to the plasma source
2. The total mass of the material is significantly lower and therefore there is less mass to "dilute" the voxels with higher activity values
3. The material composition is different



(a) Material 1 (b) Material 2

Figure 21 - Package radwaste parameters depending on material, 1e6s

When planning a radwaste packaging strategy we must consider that it is unlikely that extremely big amounts of materials will be placed into a single package, the packages shown for this model have reached more than 100 tonnes. The use of the F4E-Radwaste tool GUI allows the analysis of several packaging scenarios and its impact on the radwaste classification on-the-fly. In Figure 22 two different packages are defined for Material 1 at 1e6 seconds of decay time. Package (a) covers the whole cylinder up to a height of 20 cm, package (b) does the same but increasing the height up to 40 cm. The mass from (a) to (b) doubles while the IRAS value is reduced by around 47%. The lowest-height layers of material, closer to the plasma, are activated the most. Adding more mass from higher layers "dilutes" the specific activity of the isotopes, lowering their contribution to the IRAS and the chance of exceeding an LMA limit. Package (b) sees the activity of H3, Mn54 and Mo93 reduced enough to fall below their LMA limit. However, the amount of Nb94 determines a classification of Type B for both packages. This classification is higher than the one seen in Figure 21 (a) where the mass of Material 1 as a while received a class of Type A.



(a) Package height 20 cm (b) Package height 40 cm

Figure 22 – Package radwaste parameters depending on package size, Material 1, 1e6s

The differences in mass and radwaste class depending on the radwaste strategy shown in this section highlight the potential for optimization opened using F4E-Radwaste. Studies of more complex systems with many different materials and a significant neutron flux gradient are likely to benefit from this methodology the most.

8. Conclusions

The F4E-Radwaste methodology and tool have been designed and built to automate the analysis of nuclear systems from the perspective of activation and radwaste management. The regulatory principles, overall process, and necessary steps to perform a radwaste assessment for a given ITER system have been presented and described. A review of the different software codes, how to obtain them, install them and use them has been introduced when appropriate.

The application case of the methodology and tools to the ITER 1D benchmark has been shown, demonstrating the potential of this kind of 3D analysis.

The F4E-Radwaste capabilities greatly facilitate the production of valuable design information (3D and time-dependent distributions of the relevant activation parameters, waste amounts, decay times for de-categorisation, etc) and documentation (radwaste checklist). They also provide means for the visualisation of such information and for its processing into waste packages, thereby enabling detailed studies supporting the planning and optimisation of decommissioning activities.

New cases of application are being considered including a global estimation of the radwaste generation throughout the whole reactor employing a coarse superimposed mesh

9. Acknowledgments

Thanks to UNED as an organization and especially to Patrick Sauvan and Javier Alguacil for their developments of D1SUNED and R2SUNED and the help provided when problems arose. Their contributions are a key part of this methodology.

Appendix A – Preparation of irradiation scenarios

The irradiation scenario for the activation calculation is defined in the **irradiation_scenario.dat** file. An example of such file is presented in Figure 23. More concretely, it shows the irradiation scenario used at the ITER 1D benchmark assessment included in this document.

The recommended approach for the preparation of a new irradiation scenario is to modify a working file like that of Figure 23. The **Source Factor** keyword indicates the intensity of the source in neutrons per second, in this case the 360-degree, 500 MW plasma of ITER. Then the rest of the file consists of a table of 3 columns: **DeltaT**, **Power** and **Output required**. Each row of the table represents a phase which lasts the value of the first column in units of seconds with a constant power. The power is represented in the second column as a factor that is multiplied by the **Source Factor** value. The first row of the table in Figure 23 would then represent a phase of 6.3072e7 seconds with an intensity of 9.517752e+17 neutrons per second or 2.68 MW of thermal power.

The last column has a value of 0 unless the **DeltaT** value of the row is intended to be used as one of the decay times specified in the R2SUNED input file, then the value should be 1. All the decay times in the R2SUNED input are counted since the last irradiation phase (non-zero) power, they are not counted sequentially. In the **irradiation_scenario.dat** however, the decay times inputted are sequential phases and therefore the time spent on each must be calculated.

As an example, in the ITER 1D benchmark there were 5 decay times: 1, 2, 5, 10 and 20 years. Consequently, the first row with a value of 1 in the third column has a time delta of 3.1536e7 seconds, which equals to 1 year. The second row that represents the second decay time has the same delta time value, as 1 year must pass after the previous phase to reach a total of 2 years of decay time. The third delta time value is 9.4608e7 seconds which translates to 3 year, the 3 years need after the first 2 to reach a decay time of 5 years. The same process is followed for the rest of the decay times.

```
Source Factor
1.7757e20
DeltaT   Power    Output required
6.3072000e+07  5.3600000e-03   0
3.1536000e+08  4.1200000e-02   0
2.1034512e+07  0.0000000e+00   0
4.1785200e+07  8.3000000e-02   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.0000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.4000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.4000000e+00   0
3.9200000e+03  0.0000000e+00   0
4.0000000e+02  1.4000000e+00   0
3.1536000e+07  0.0000000e+00   1
3.1536000e+07  0.0000000e+00   1
9.4608000e+07  0.0000000e+00   1
1.5768000e+08  0.0000000e+00   1
3.1536000e+08  0.0000000e+00   1
```

Figure 23 - irradiation_scenario.dat file example

Appendix B – Modification of PHOTON.dat file (isotope list)

The **PHOTON.dat** file is found in the **common_data** folder inside **R2SUNEDV2** as seen in Figure 2. It contains all the names of the isotopes that will be tracked in the R2SUNED activation calculation. Figure 24 shows a detail of the contents of the file.

For each isotope there are two lines.

The first line of an isotope presents:

1. Atomic number of the isotope
2. Nuclide name
3. A value of 1 (represents the number of gamma lines to consider for the isotope)

Unfortunately, the formatting of this line is tricky, and the calculation will crash if there is an extra or missing whitespace. The element name may include an **M** or **N** character to indicate an isomer and the number of characters of the element name or the number of digits of the atomic number seem to alter the formatting rules.

The second line is always the same, “1.0000E+00 1.0000E+00”. It represents a gamma energy of 1 MeV and a probability for that gamma of 1. This artificial data is used as we are only interested in the activity of each isotope, not the gamma energies or probabilities.

Due to the difficulty of conforming to the required format, a Python script has been prepared to aid in this task. It can be found inside the resources folder of the F4E-Radwaste tool.

```
43  TC 99         1
1.0000E+00 1.0000E+00
44  RU103         1
1.0000E+00 1.0000E+00
44  RU106         1
1.0000E+00 1.0000E+00
45  RH101         1
1.0000E+00 1.0000E+00
45  RH102         1
1.0000E+00 1.0000E+00
45  RH102M        1
1.0000E+00 1.0000E+00
```

Figure 24 - Example of the contents of PHOTON.dat file

Appendix C – Considerations regarding the combination of CuV data points

During the last steps of the F4E-Radwaste methodology the activity data is combined in different ways. The data may be combined in a per-component basis, a material basis, or a package basis. In any of those cases it usually is needed to combine several data points and collapse them into a single value for a specific voxel. In this context a data point refers to a set of values that corresponds to a specific location. The isotope activity of the portion of Cell X found inside Voxel Y at decay time Z would be an example of data point.

To combine several data points, a simple average or sum would be incorrect. The radwaste parameters depend on the specific activity of the isotopes which in turn will be affected not only by the specific activity of each data point but also its associated mass. Whenever data points are combined via the F4E-Radwaste tool the following steps are taken:

1. The relevant data points are identified depending on the type of post-processing and filtering applied
2. The absolute activity of all relevant data points is summed, its units are in Bq
3. The mass of all relevant data points is summed, its units are in grams
4. The total absolute activity of each isotope is divided by the total mass, units are now in Bq/g
5. The radwaste relevant parameters are calculated via the specific activity values and the radwaste classification criteria is applied

For example, Cell 1, Cell 2, and Cell 3 appear in the Voxel 32, that voxel contains a mass of 20 grams of Cell 1, 45 grams of Cell 2 and 10 grams of Cell 3. The absolute activity of each cell respectively for isotope Fe55 is 10, 20 and 30 Bq. Cells 1 and 2 are made of Material 100 while Cell 3 is made of Material 300. In this post-processing, we are combining the data on a material basis.

Processing of Material 100 in Voxel 32:

1. Cells 1 and 2 are identified
2. Total activity of Fe55 = 10 + 20 = 30 Bq
3. Total mass = 20 + 45 = 65 grams
4. Specific activity of Fe55 = 30 / 65 = 0.46 Bq/g
5. The contribution to the IRAS of Fe55 can now be calculated, its LMA limit can be checked

Processing of Material 300 in Voxel 32:

1. Cell 3 is identified
2. Total activity of Fe55 = 30 Bq
3. Total mass = 10 grams
4. Specific activity of Fe55 = 30 / 10 = 3 Bq/g
5. The contribution to the IRAS of Fe55 can now be calculated, its LMA limit can be checked

Appendix D – Dose rates calculation

The F4E_radwaste tool can calculate dose at 1 meter and contact dose rate (CDR) for the packages generated with the GUI and for each component when using the **by component processing**. The calculation is performed by multiplying the activity of each isotope with a set of dose factors obtained from [R16]. Please refer to [R17] for a detailed explanation of the calculation process.

The factors for the CDR calculation depend on the element composition of the material mix of the component/package because of the self-shielding and built-up effects. When performing a **by component processing**, the CDR factors are calculated individually for each component. The isotope composition of every cell belonging to the component is identified and compounded into a new component-wise element mix.

The CDR factors of the M200 material (ordinary concrete) from E-Lite have been calculated and hard-coded into the tool. These factors are used when calculating the CDR for a GUI-defined 3D package. That is, it is considered that the self-shielding material of 3D packages is always concrete. This decision was taken because of the cementing process in which concrete is poured on the Type A containers. Furthermore, containers of this type usually also have inner concrete walls.

The dose rate values provided by this calculation can be considered conservative. The concrete of the cementing process and walls is *diluting* the specific activity of the container, usually by a factor of 2. This dilution is not considered in the calculation.

The activity of the geometry during the calculation of the dose at 1 meter is virtually collapsed into a *source point*. This approximation is reasonable for the smaller components. The values for the more massive components provide a clearly conservative estimate.

The results of the CDR calculation may be locally conservative depending on the geometry, size, and distribution of the activation as a semi-infinite homogeneous slab is considered.