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# Deterministic Time-Dependent Neutron Transport Benchmark without Spatial Homogenization

(C5G7-TD)

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#### 1. Introduction

Increasing efforts have been made to the development of codes for transient calculations of nuclear reactors in recent years. In order to ensure reliable modeling of neutron physics within a state-of-the-art transient code, the neutron kinetics part of such a code should be based on the full-scale calculation of the space-time neutron kinetics equations without use of the diffusion approximation and spatial homogenization. Such advanced approaches require the verification of neutron kinetics program modules through the cross-verification of codes, which are used to calculate thoroughly defined test cases, or the benchmarks.

However, existing benchmark problems are not able to satisfy the demand for verifying codes/methods for performing the homogenization-free time-dependent transport calculations. On one hand, some of them are simplified diffusion benchmarks, in which the computational domain is composed of several homogeneous regions. On the other hand, some of them have a broad range of sources of uncertainties involved in the calculation, such as the nuclear data, group cross section preparation procedure, and potentially other computational simplifications, making it difficult to reveal methodical errors of space-time neutron kinetics codes.

The main objective of this benchmark is to specify a series of space-time neutron kinetics test problems with heterogeneous domain description for solving the time-dependent group neutron transport equation without feedbacks. Physical materials in these benchmarks are described by transport macroscopic cross sections. Such benchmarks would allow carrying out verification of developed deterministic codes and rigorously revealing methodical errors. Moreover, such benchmarks would allow studying possible inaccuracy of spatial homogenization and diffusion approximation in time-dependent cases. After the completion of the proposed kinetics benchmark it will be extended to more realistic dynamics benchmark, which will take into account the thermal-hydraulic feedback mechanisms.

This benchmark has been approved by Organization for Economic Cooperation and Development Nuclear Energy Agency (OECD/NEA) Nuclear Science Committee (NSC) Working Party on Scientific Issues in Reactor Systems (WPRS) in the meeting in February 2015.

#### 2. Benchmark model specification

#### 2.1 Core description

The current benchmark model is based on the well-studied steady-state C5G7 benchmark problems, which were developed to test the capabilities of radiation transport codes that do not utilize spatial homogenization above the fuel pin level [1-3]. It is a miniature light water reactor (LWR) with sixteen fuel assemblies (minicore): eight uranium oxide (UO<sub>2</sub>) assemblies and eight mixed oxide (MOX) assemblies, surrounded by a water reflector. It features a quarter-core radial symmetry in the 2-dimensional (2-D) configuration, as depicted in Figure 1. Note that the four assemblies in this representation are numbered 1-4 for the convenience of the following specification.

Both  $UO_2$  and MOX assemblies follow the  $17 \times 17$  configuration, consisting of 264 fuel pins, 24 guide tubes for control rods and one instrument tube for a fission chamber in the center grid-cell. All pin cells have a pin radius of 0.54 cm with a pitch of 1.26 cm. The pin cell layout for the south-east quadrant is depicted in Figure 2. It can be seen that the MOX assemblies have three enrichments of 4.3%, 7.0%, and 8.7%.

The C5G7 benchmark provided the transport corrected few-group cross sections and scattering matrices in seven-group structure for UO<sub>2</sub>, MOX (three enrichments), the guide tubes and fission chamber, and the moderator described in the problem specification. These cross sections, as listed in Table 1 through Table 7 in Appendix I, were obtained from transport lattice calculations using the collision probability code DRAGON [4] and the WIMS-AECL 69 group library at constant room temperature (20 °C). In DRAGON calculations, standard flux weighting was used to collapse cross sections to seven energy groups and to homogenize fuel, gap, and cladding materials into homogenized fuel compositions. The seven-group moderator, homogenized guide tube, control rod, and fission chamber cross sections were obtained using a UO<sub>2</sub> fuel spectrum. In another word, all cross sections were provided for all the pin cells in a simplified 2-region geometry, as shown in Figure 3, where "Zone 2" represents the moderator outside the outer tube and "Zone 1" refers to the mixture of all medium surrounded by "Zone 2". It is advised to treat the fission spectrum provided in tables as the cumulative spectrum, which is defined in Appendix IV.

The geometric configuration and isotopic composition of the materials, based on which the few-group cross sections were generated, are also provided in Appendix II [1]. Participants are thus given the choice of either directly using the provided macroscopic cross sections, or generating their own group constants to better meet the requirements of their solution methods, such as energy group structure, etc. Reference continuous-energy and multi-group Monte Carlo calculations can be performed based on these specifications. The nuclide densities could also be used to perform Uncertainty and Sensitivity (U/S) analysis by propagating microscopic cross section uncertainties through the typical calculation chain of core calculations [5]. The benchmark team will contribute further to the specification by generating group-constants with SCALE 6.1 and SCALE 6.2 (using ENDF/B-VII.1) based on the specified nuclide densities. It is suggested that participants who perform the heterogeneous calculation for cross section generation should model the pin cell with double cladding exactly.

The control rod configuration was later introduced in the 3-D extension case of C5G7 benchmark [6]. The control rod macroscopic cross sections, presented in Table 8, obtained using the UO<sub>2</sub> cell spectrum. The pin cell geometry was based on the guide tube cell model given in Table 14, assuming no gap between the control rod and cladding. The 3-dimensional (3-D) geometry is adopted in the current benchmark with minor modifications, primarily on the axial core configuration. The height of the fuel assembly is increased to 128.52 cm with additional 21.42-cm-thick upper and lower axial reflector. Vacuum boundary condition has been applied to the axial boundary of the core so that control rods can only be inserted from the top. Figure 4 gives the new dimensions of the 3-D geometry where the pin cell (Figure 3) and assembly layout (Figure 1) of reference [1] have been maintained.

Part of the preparation effort for the benchmark specification is related to the generation of required kinetics parameters, including delayed neutron fractions, delayed neutron precursor decay constants, delayed

neutron group spectra, and group neutron velocities. Various models have been examined and implemented to produce these parameters [7]. The resulting parameters evaluated in 8 delayed neutron groups are, as shown in Table 9 through Table 11, based on the data in [8]. It should be noted that the WIMS-D energy group boundaries were chosen for the kinetics parameters calculation, because it is the closest to the energy structure (ANL structure, see Table 12) that was used to generate the seven-group cross sections [9]. Table 13 shows the average neutron velocity for various fuel compositions based on this group structure. It is left to the participants to decide to use either provided data or their self-generated kinetics parameters in their calculations.

There are two sets of exercises considered in this problem. The first set, which consists of 3 exercises, is focused on the 2-D configuration of the C5G7 core. The second set, including 2 exercises, is with regard to the 3-D C5G7 configuration. The detailed perturbation law of each exercise is described in the following sections. Accurate multi-group Monte Carlo reference solutions will be obtained for all configurations.

#### 2.2 2-D transient problems

The 2-D time-dependent benchmark, including four transient exercises featured with control rod cluster movement and moderator density change with various rate and magnitude, is based on the 2-D configuration of the C5G7 core, as shown in Figure 1.

### **2.2.1** Exercise 0 (TD0)

Exercise 0 of this time-dependent benchmark problem (TD0) is focused on the simulation of a postulated control rod insertion and withdrawal event. It is assumed that all control rods are fully removed from the core initially, and the transient is initiated by an abrupt control rod insertion (one rod bank per fuel assembly) for a depth equivalent to 10% of the active core height at time 0. The control rod stays still until the end of 1 s, when it extracted by half of the inserted length and maintains the position for another second. All the inserted rod banks are withdrawn to their initial positions at the end of 2 s. It is assumed that all rod bank movements take place instantaneously.

This postulated transient event can be approximated in the 2-D calculations as a step change of the material composition, i.e., an instantaneous replacement of the moderator-filled guide tube material by the control rod material in Zone 1 of the affected cells, as shown in the black line in Figure 5. Eq. (1) gives the mathematical expression of the cross section mixing.

$$\begin{split} & \Sigma_{x}(t) = \Sigma_{x}^{GT}, t = 0, t \geq 2s \\ & \Sigma_{x}(t) = \Sigma_{x}^{GT} + 0.1(\Sigma_{x}^{R} - \Sigma_{x}^{GT}), 0 < t \leq 1s \\ & \Sigma_{x}(t) = \Sigma_{x}^{GT} + 0.05(\Sigma_{x}^{R} - \Sigma_{x}^{GT}), 1s \leq t < 2s \end{split} \tag{1}$$

where  $\Sigma$  refers to the seven-group macroscopic cross sections, the superscription "R" and "GT" stands for the domain of control rod and guide tube, respectively. The subscription "x" is denoted as the reaction type, which includes absorption and scattering.

There are 5 test problems in TD0, as listed below, that differ from each other on the location where the control rod movements occur.

- TD0-1: insertion/withdrawal of bank 1.
- TD0-2: insertion/withdrawal of bank 3.
- TD0-3: insertion/withdrawal of bank 4.
- TD0-4: insertion/withdrawal of banks 1, 3, and 4 simultaneously.
- TD0-5: insertion/withdrawal of banks 1-4 simultaneously.

The required output parameters as well as the duration and time step size of TD0 simulations can be found in Sec 3.1.

# 2.2.2 Exercise 1 (TD1)

Exercise 1 (TD1) is also concerned with control rod insertion and extraction transient, starting from the unrodded core condition, while the difference from TD0 is that all rod banks move at a constant speed. To start the transient, one or more control rod banks (one rod bank per fuel assembly) are inserted to depth equal to 1% of the total core height within 1 s. During the next 1 s all the inserted rod banks are withdrawn to their initial positions.

This postulated transient event can be approximated in the 2-D calculations as a ramp change of the material composition, i.e., a linear replacement of the moderator-filled guide tube material by the control rod material in Zone 1 of the affected cells, as shown in blue line in Figure 6. More specifically, the weight of the control rod cross section in the mixture linearly increases from 0 to 0.01 during the initial 1 s, then return to 0 for another 1 s. This can be written as the following:

$$\Sigma_{x}(t) = \Sigma_{x}^{GT} + 0.01(\Sigma_{x}^{R} - \Sigma_{x}^{GT})t, 0 \le t < 1s$$

$$\Sigma_{x}(t) = \Sigma_{x}^{GT} + 0.01(\Sigma_{x}^{R} - \Sigma_{x}^{GT})(2 - t), 1s \le t < 2s$$

$$\Sigma_{x}(t) = \Sigma_{x}^{GT}, t \ge 2s$$
(2)

where the definition of each component is the same as in Eq. (1). There are 5 test problems in this exercise, as listed below, which vary from each other on the location where the control rod movements occur.

- TD1-1: insertion/withdrawal of bank 1.
- TD1-2: insertion/withdrawal of bank 3.
- TD1-3: insertion/withdrawal of bank 4.
- TD1-4: insertion/withdrawal of banks 1, 3, and 4 simultaneously.
- TD1-5: insertion/withdrawal of banks 1-4 simultaneously.

The order of these test problems by increasing the maximum reactivity inserted is: TD1-3, TD1-2, TD1-1, TD1-4, and TD1-5. The required output parameters as well as the duration and time step size of TD1 simulations is specified in Sec 3.1.

#### **2.2.3** Exercise 2 (TD2)

Exercise 2 of the current benchmark problem (TD2) is designed to simulate a control rod transient that is very similar to TD1, but with a different depth (or magnitude) of the control rod insertion. In TD2, the maximum depth that the control rods can reach 1 second after the transient starts is 10% of the total core height. All control rods are at fully withdrawn position at the end of the transient (2 seconds). Again, the control rod insertion/withdraw happens in a linear manner, as shown in red line in Figure 6.

As a result, the modification of the mixture cross section in Zone 1 in TD2 differs from that of TD1 by adjusting the weight of mixture cross section to 0.1 and 0.9 for control rod and guide tube, respectively, after 1 s into the transient. This perturbation law can be written in the expression of Eq. (3):

$$\Sigma_{x}(t) = \Sigma_{x}^{GT} + 0.1(\Sigma_{x}^{R} - \Sigma_{x}^{GT})t, 0 \le t < 1s$$

$$\Sigma_{x}(t) = \Sigma_{x}^{GT} + 0.1(\Sigma_{x}^{R} - \Sigma_{x}^{GT})(2 - t), 1s \le t < 2s$$

$$\Sigma_{x}(t) = \Sigma_{x}^{GT}, t \ge 2s$$
(3)

There are three test problems in TD2 exercise, as listed below.

- TD2-1: insertion/withdrawal of bank 1.
- TD2-2: insertion/withdrawal of bank 3.
- TD2-3: insertion/withdrawal of bank 4.

The required output parameters as well as the duration and time step size of TD2 simulations can be found in Sec 3.1.

#### **2.2.4** Exercise 3 (TD3)

The third exercise (TD3) is intended as a simulation of a transient event of the change of core moderator density. It is assumed that the moderator density in all fuel assemblies is at its nominal value as the starting point, and starts to decrease linearly before reaching its minima after 1 s into the transient. This minimum value is represented as a fraction, denoted as  $\omega$  ( $0 \le \omega \le 1$ ), of its initial value. The moderator density then linearly returns to its initial value within next 1 s. It should be noted that this change mechanism affects all cells in the core uniformly but the water density in the reflector is not affected.

The simulation of TD3 transient can be achieved by the linear perturbation of the moderator cross sections, as shown in Zone 2 of Figure 3, of all cells across the core. At the end of 1 s, all cross sections are equal to certain fraction of their initial values. The perturbation continues by the linearly increasing these cross sections to their initial values during another 1 s.

There are four test problems in TD3, as listed below, each with its own value of  $\omega$  varying from 0.80 to 0.95. The rate of change of moderator density for each of these test problems is illustrated in Figure 7.

- TD3-1:  $\omega = 0.95$ .
- TD3-2:  $\omega = 0.90$ .
- TD3-3:  $\omega = 0.85$ .
- TD3-4:  $\omega = 0.80$ .

Sec 3.1 gives the output parameters of interest, the duration and time step size of TD3 simulations.

# 2.3 3-D transient problems

The 3-D time-dependent benchmark adopts the 3-D configuration of the C5G7 core, as shown in Figure 4. Two exercises are defined to simulate transient events including control rod insertion/withdrawal and moderator density change with various rate and magnitude.

#### **2.3.1** Exercise 4 (TD4)

The TD4 exercise is driven by the control rod insertion/withdrawal transient in the 3-D core configuration. An initial core condition, referred to as the Unrodded case, is first defined, where the control rod banks (one bank for each assembly) are inserted into the upper axial water reflector as indicated by the shading in Figure 4. Figure 8 shows a slice in the radial configuration in the top reflector, including the control rod banks, fission chamber and moderator. It is suggested that the fission chambers and control rods present in the axial reflector region should be modelled.

It is assumed that the rod bank moves at a constant speed, which allows it to be fully inserted into the assembly from the fully withdrawn position within 6 s. Note that this is a hypothetic value proposed only for the purpose of reducing the computational effort in the transient calculation.

There are 5 test problems defined in the TD4 exercise in total and their scenarios are described in Figure 9. Examples of understanding these figures are given below. The transient of TD4-1 is initiated by the rod bank insertion of Assembly No 1, and within 2 s the rod bank is inserted 1/3 way into the fuel assembly. After that, the control rod bank is withdrawn at the same speed and the core configuration returns to its initial Unrodded state at the end of 4 s.

TD4-3 transient is initiated by inserting the rod bank 3 at a constant speed and after 2 s into the transient the rods of Assembly No 1 are inserted at the same speed. At the end of 4 s both rod banks 1 and 3 are withdrawn until the core condition returns to the Unrodded configuration.

TD4-5 transient is initiated by inserting the rod bank 1, and after 2 s into the transient the withdrawal of rod bank 1 and insertion of rod bank 3 starts simultaneously. At the end of 4 s, the rod bank 1 is fully withdrawn, while bank 3 is inserted 1/3 way into the fuel assembly and will stay in this position for another 2 s before the withdrawal. All rods will be removed from the core at the end of 8 s. To summarize, the 5 test problems in TD4 exercise are:

- TD4-1: bank 1 insertion/withdrawal.
- TD4-2: bank 3 insertion/withdrawal.
- TD4-3: bank 1 and 3 insertion/withdrawal.
- TD4-4: bank 3 and 4 insertion/withdrawal.
- TD4-5: bank 1 and 3 insertion/withdrawal.

Sec 3.2 specifies the output parameters of interest as well as the duration and time step size of TD4 simulations.

# 2.3.2 Exercise 5 (TD5)

The exercise 5 (TD5) models a series of moderator density change transient events. It is assumed that all control rods are positioned in the fully withdrawn position (Unrodded configuration) throughout the transient and the moderator density is at the nominal level at the starting point. Totally 4 test problems have been defined for various transient mechanisms by varying the rate and location of moderator density change, as shown in Figure 10.

For example, TD5-1 transient is initiated by the moderator density decrease in Assembly No 1 at the constant rate of 5% per second, and after 1 s into the transient the moderator density in Assembly No 3 starts to drop at the same rate. The moderator density starts to increase right after 2 s into the transient in both assemblies at the rate of 5% per second, and it returns to the nominal value within another 2 s and 1 s respectively for Assembly No 1 and 3, separately. The moderator density in Assembly No 2 and 3 is not affected in this transient. Note that all the density change is expected to take place uniformly with the assembly, that is, no spatial dependence is assumed.

To summarize, the 4 test problems in TD5 exercise are:

- TD5-1: moderator density change in Assembly No 1 and 3.
- TD5-2: moderator density change in Assembly No 1 and 3.
- TD5-3: moderator density change in Assembly No 1, 3, and 4.
- TD5-4: moderator density change in Assembly No 2, 3, and 4.

It is worth mentioning that the water density in both radial and axial reflector is maintained in its nominal value throughout the transient. The required output parameters as well as the duration and time step size of TD5 simulations can be found in Sec 3.2.

#### 3. Calculation and results

The C5G7 core in both 2-D and 3-D configurations will be supercritical using the few-group cross sections provided in Appendix I or those generated by the participants. It is suggested that the initial state for each exercise should be made critical by adjusting the neutron production uniformly in all fuel regions; that is, dividing Nu by the core  $k_{\text{eff}}$ .

In addition to the solution method to the time-dependent transport equation, difference may rise in the comparison of transient solutions due to the deviation of provided and self-generated few-group cross sections and kinetic parameters. Participants who utilize self-generated data are thus encouraged to perform additional calculations using provided data to help quantify the impact of the difference in input data on the final solution.

In order to fully capture the temporal behavior of the core during the postulated transients, simulations should be performed with sufficiently small time step size, especially at the beginning of the events. Although it is up to the participants to determine the time discretization scheme based on the requirement of their codes, the resulting scheme should comply with the time points at which output parameters are required, which can be found in the output template provided by the benchmark team. It is worth mentioning the time point configuration is dependent on both transient case and required output parameters. In principle, the time step should be no longer than 25 ms during the transient but could be increased gradually towards the end of simulation.

#### 3.1 2-D transient problems

The first set of exercises, including TD0, TD1, TD2, and TD3 cases, is focused on the transient solutions of the 2-D configuration of the C5G7 core. The mixing process mentioned in Sec 2.2.1, in principle, should also involve the group neutron velocity, which is dependent on both time and space (fuel zone location) and their initial values are given in Table 13 for various types of materials. Participants have the permission to decide the treatment of the dependency of neutron velocity on time and space during the 2-D transients, since its impact on the transport solution is considered small. The simplest approximation would be to completely ignore this dependency, that is, to use a single set of group neutron velocity for all materials throughout the transient. However, any approximation applied for obtaining the solution should be reported along with the results submittal for the purpose of understanding its influence on the numerical solution.

The simulation time of the 2-D transient problem is set to be 10 s for all cases. The following parameters of interest will be requested for the initial steady state and at the specified time points:

- Core dynamic reactivity.
- Fractional total core fission rate: the fraction of total core fission rate to its initial value at t = 0. The fission rate in the fission chamber should be neglected.
- Effective delayed neutron fraction.
- Prompt neutron life time.
- Radial distribution of axially integrated fission rate on the fuel assembly basis.
- Radial distribution of axially integrated fission rate on the pin-by-pin basis.

The fission rate distribution should be normalized in such a way that the values of all assemblies (or pin cells) across the core is summed up to the ratio of total core fission rate at a given time point to that of the beginning of the transient. The summation of the distribution is therefore 1.0 at time t = 0.

# 3.2 3-D transient problems

It is suggested that participants will simulate cases in TD4 and TD5 for 16 s and 12 s, respectively. As for the output, similar "core integral" parameters are required at the specified time points:

- Core dynamic reactivity.
- Fractional total core fission rate: the fraction of total core fission rate to its initial value at t = 0. The fission rate in the fission chamber should be neglected.
- Effective delayed neutron fraction.
- Prompt neutron life time.

The method for normalization of the fission rate distribution is the same as that in 2-D cases.

In addition, at various time points the 3-D distributions of normalized fission rate on both assembly and pin level are requested as a series of core maps that correspond to different axial layers in the active core. Those snapshots of 3-D map with resolution level of pin cell and assembly will be used to generate the axially and radially integrated 2-D distribution. The requested axial locations will be measured by distance from the bottom of the core and will be specified for each case in the templates for results' submission.

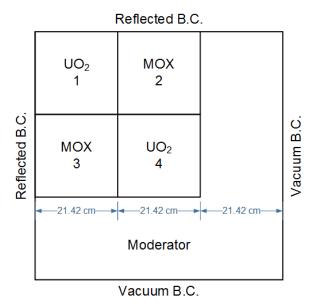


Figure 1. 2-D configuration for the C5G7 benchmark problem

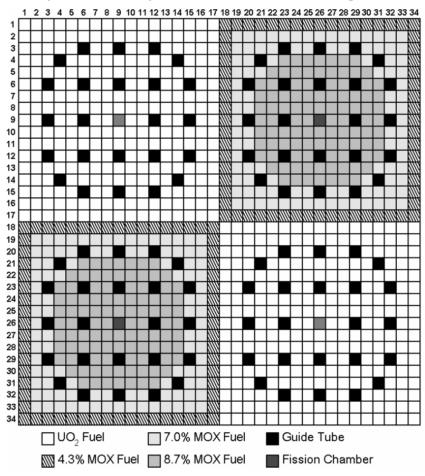


Figure 2. C5G7 fuel pin compositions and numbering scheme

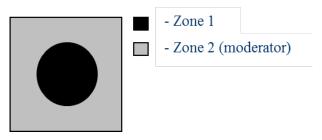


Figure 3. C5G7 pin cell layout

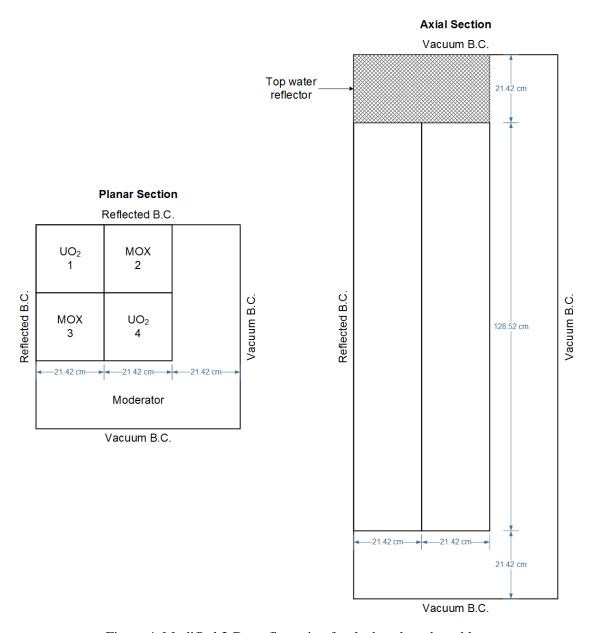


Figure 4. Modified 3-D configuration for the benchmark problem

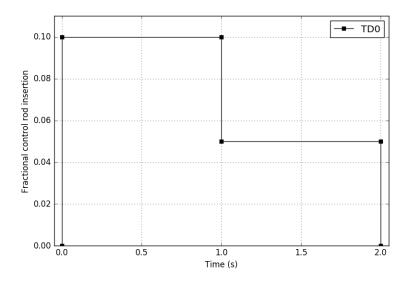


Figure 5. Control rod movement in TD0 transient exercise

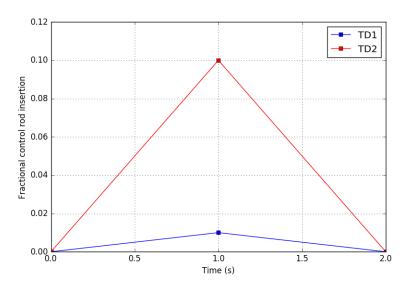


Figure 6. Control rod movement in transient exercise TD1 and TD2

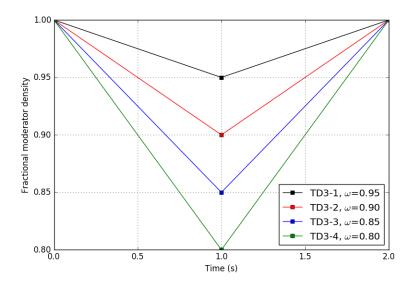


Figure 7. Core average moderator density change in TD3 exercises

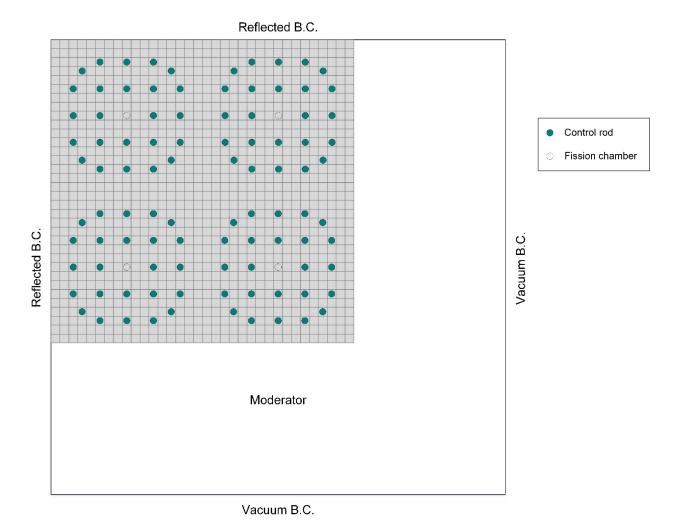


Figure 8. Geometry configuration for the top water reflector

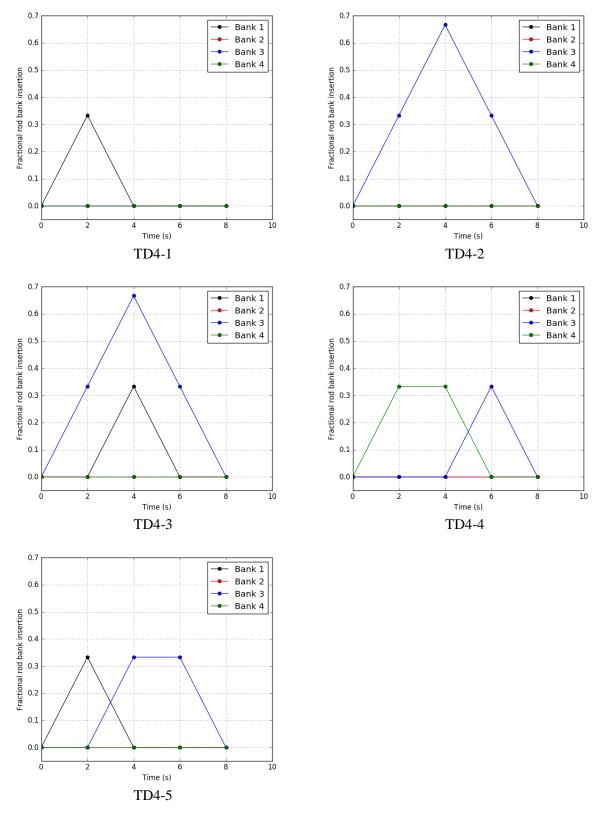


Figure 9. Relative depth of control bank movement in TD4 exercise

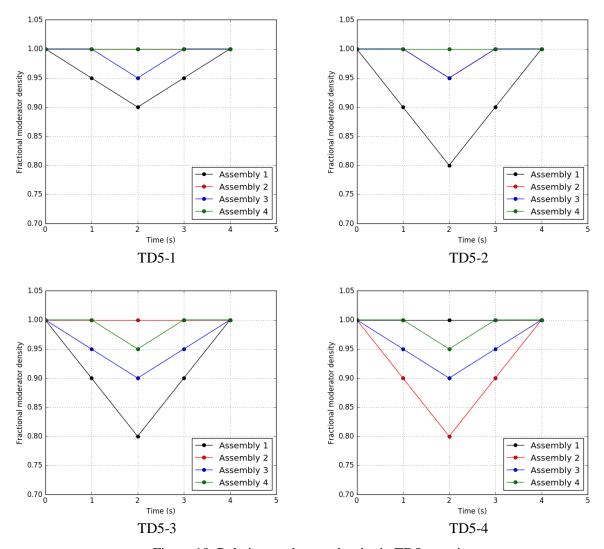


Figure 10. Relative moderator density in TD5 exercise

#### References

- 1. C. Cavarec, J. Perron, D. Verwaerde and J. West, "The OECD/NEA benchmark calculations of power distributions within assemblies," Electricity de France, 1994.
- 2. S. Cathalau, J. Lefebvre and J. West, "Proposal for a second stage of the benchmark on power distributions within assemblies," in NEA/NSC/DOC (1996) 2, Moscow, Nuclear Energy Agency, 1996.
- 3. E. Lewis, M. Smith, N. Tsoulfanidis, G. Palmiotti, T. Taiwo and R. Blomquist, "Benchmark specification for Deterministic 2-D/3-D MOX fuel assembly transport calculations without spatial homogenization (C5G7 MOX)," NEA/NSC, 2001.
- 4. G. Marleau, A. Hebert and R. Roy, "A User's Guide for DRAGON," IGE-174, Rev, vol. 3, 1996.
- 5. M. Zilly, K. Velkov, W. Zwermann, Y. S. Jung and H. G. Joo, "Quantifying nuclear data uncertainty in nTracer simulation results with the XSUSA method," in ANS MC2015 Joint International Conference on Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method, Nashville, TN, 2015.
- 6. M. A. Smith, E. Lewis and B.-C. Na, "Benchmark on Deterministic Transport Calculations Without Spatial Homogenization (MOX Fuel Assembly 3-D Extension Case)," Organization for Economic Co-Operation and Development/Nuclear Energy Agency Report NEA, 2005.
- 7. V. F. Boyarinov, A. E. Kondrushin and P. A. Fomichenko, "Benchmark on deterministic time-dependent transport calculations without spatial homogenization," in PHYSOR 2014 The Role of Reactor Physics Toward a Sustainable Future, Kyoto, Japan, September 28 October 3, 2014.
- 8. G. Rudstam, P. Finck, A. Filip, A. D'Angelo and R. McKnight, "International Evaluation Co-operation. Volume 6: Delayed neutron data for the major actinides," NEA/WPEC-6 Report, 2002.
- 9. C. Bergiers, B. Ivanov and K. Ivanov, "Establishment of consistent benchmark framework for performing high-fidelity whole core transport/diffusion calculations," in International Conference on Advances in Nuclear Reactor Simulations, PHYSOR 2006, Vancouver, BC, Canada, 2006.

# Appendix I Macroscopic cross sections and kinetics parameters

Table 1. UO<sub>2</sub> fuel-clad macroscopic cross sections

Group	Transport cross section (cm <sup>-1</sup> )	Absorption cross section (cm <sup>-1</sup> )	Capture cross section (cm <sup>-1</sup> )	Fission cross section (cm <sup>-1</sup> )	Nu	Chi
1	1.77949E-01	8.02480E-03	8.12740E-04	7.21206E-03	2.78145E+00	5.87910E-01
2	3.29805E-01	3.71740E-03	2.89810E-03	8.19301E-04	2.47443E+00	4.11760E-01
3	4.80388E-01	2.67690E-02	2.03158E-02	6.45320E-03	2.43383E+00	3.39060E-04
4	5.54367E-01	9.62360E-02	7.76712E-02	1.85648E-02	2.43380E+00	1.17610E-07
5	3.11801E-01	3.00200E-02	1.22116E-02	1.78084E-02	2.43380E+00	0.00000E+00
6	3.95168E-01	1.11260E-01	2.82252E-02	8.30348E-02	2.43380E+00	0.00000E+00
7	5.64406E-01	2.82780E-01	6.67760E-02	2.16004E-01	2.43380E+00	0.00000E+00

Scattering block (unit: cm<sup>-1</sup>)

Group	To Group 1	To Group 2	To Group 3	To Group 4	To Group 5	To Group 6	To Group 7
1	1.27537E-01	4.23780E-02	9.43740E-06	5.51630E-09	0.00000E+00	0.00000E+00	0.00000E+00
2	0.00000E+00	3.24456E-01	1.63140E-03	3.14270E-09	0.00000E+00	0.00000E+00	0.00000E+00
3	0.00000E+00	0.00000E+00	4.50940E-01	2.67920E-03	0.00000E+00	0.00000E+00	0.00000E+00
4	0.00000E+00	0.00000E+00	0.00000E+00	4.52565E-01	5.56640E-03	0.00000E+00	0.00000E+00
5	0.00000E+00	0.00000E+00	0.00000E+00	1.25250E-04	2.71401E-01	1.02550E-02	1.00210E-08
6	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.29680E-03	2.65802E-01	1.68090E-02
7	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.54580E-03	2.73080E-01

Table 2. 4.3% MOX fuel-clad macroscopic cross sections

	Transport	Absorption	Capture	Fission		
Group	cross section	cross section	cross section	cross section	Nu	Chi
	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )		
1	1.78731E-01	8.43390E-03	8.06860E-04	7.62704E-03	2.85209E+00	5.87910E-01
2	3.30849E-01	3.75770E-03	2.88080E-03	8.76898E-04	2.89099E+00	4.11760E-01
3	4.83772E-01	2.79700E-02	2.22717E-02	5.69835E-03	2.85486E+00	3.39060E-04
4	5.66922E-01	1.04210E-01	8.13228E-02	2.28872E-02	2.86073E+00	1.17610E-07
5	4.26227E-01	1.39940E-01	1.29177E-01	1.07635E-02	2.85447E+00	0.00000E+00
6	6.78997E-01	4.09180E-01	1.76423E-01	2.32757E-01	2.86415E+00	0.00000E+00
7	6.82852E-01	4.09350E-01	1.60382E-01	2.48968E-01	2.86780E+00	0.00000E+00

Scattering block (unit: cm<sup>-1</sup>)

Group	To Group 1	To Group 2	To Group 3	To Group 4	To Group 5	To Group 6	To Group 7
1	1.28876E-01	4.14130E-02	8.22900E-06	5.04050E-09	0.00000E+00	0.00000E+00	0.00000E+00
2	0.00000E+00	3.25452E-01	1.63950E-03	1.59820E-09	0.00000E+00	0.00000E+00	0.00000E+00
3	0.00000E+00	0.00000E+00	4.53188E-01	2.61420E-03	0.00000E+00	0.00000E+00	0.00000E+00
4	0.00000E+00	0.00000E+00	0.00000E+00	4.57173E-01	5.53940E-03	0.00000E+00	0.00000E+00
5	0.00000E+00	0.00000E+00	0.00000E+00	1.60460E-04	2.76814E-01	9.31270E-03	9.16560E-09
6	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.00510E-03	2.52962E-01	1.48500E-02
7	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.49480E-03	2.65007E-01

Table 3. 7.0% MOX fuel-clad macroscopic cross sections

	Transport	Absorption	Capture	Fission		
Group	cross section	cross section	cross section	cross section	Nu	Chi
	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )		
1	1.81323E-01	9.06570E-03	8.11240E-04	8.25446E-03	2.88498E+00	5.87910E-01
2	3.34368E-01	4.29670E-03	2.97105E-03	1.32565E-03	2.91079E+00	4.11760E-01
3	4.93785E-01	3.28810E-02	2.44594E-02	8.42156E-03	2.86574E+00	3.39060E-04
4	5.91216E-01	1.22030E-01	8.91570E-02	3.28730E-02	2.87063E+00	1.17610E-07
5	4.74198E-01	1.82980E-01	1.67016E-01	1.59636E-02	2.86714E+00	0.00000E+00
6	8.33601E-01	5.68460E-01	2.4466E-01	3.23794E-01	2.86658E+00	0.00000E+00
7	8.53603E-01	5.85210E-01	2.22407E-01	3.62803E-01	2.87539E+00	0.00000E+00

Scattering block (unit: cm<sup>-1</sup>)

Group	To Group 1	To Group 2	To Group 3	To Group 4	To Group 5	To Group 6	To Group 7
1	1.30457E-01	4.17920E-02	8.51050E-06	5.13290E-09	0.00000E+00	0.00000E+00	0.00000E+00
2	0.00000E+00	3.28428E-01	1.64360E-03	2.20170E-09	0.00000E+00	0.00000E+00	0.00000E+00
3	0.00000E+00	0.00000E+00	4.58371E-01	2.53310E-03	0.00000E+00	0.00000E+00	0.00000E+00
4	0.00000E+00	0.00000E+00	0.00000E+00	4.63709E-01	5.47660E-03	0.00000E+00	0.00000E+00
5	0.00000E+00	0.00000E+00	0.00000E+00	1.76190E-04	2.82313E-01	8.72890E-03	9.00160E-09
6	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.27600E-03	2.49751E-01	1.31140E-02
7	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.86450E-03	2.59529E-01

Table 4. 8.7% MOX fuel-clad macroscopic cross sections

	Transport	Absorption Capture		Fission			
Group	cross section	cross section	cross section	cross section	Nu	Chi	
	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )			
1	1.83045E-01	9.48620E-03	8.14110E-04	8.67209E-03	2.90426E+00	5.87910E-01	
2	3.36705E-01	4.65560E-03	3.03134E-03	1.62426E-03	2.91795E+00	4.11760E-01	
3	5.00507E-01	3.62400E-02	2.59684E-02	1.02716E-02	2.86986E+00	3.39060E-04	
4	6.06174E-01	1.32720E-01	9.36753E-02	3.90447E-02	2.87491E+00	1.17610E-07	
5	5.02754E-01	2.08400E-01	1.89142E-01	1.92576E-02	2.87175E+00	0.00000E+00	
6	9.21028E-01	6.58700E-01	2.83812E-01	3.7488E-01	2.86752E+00	0.00000E+00	
7	9.55231E-01	6.90170E-01	2.59571E-01	4.30599E-01	2.87808E+00	0.00000E+00	

Scattering block (unit: cm<sup>-1</sup>)

Group	To Group 1	To Group 2	To Group 3	To Group 4	To Group 5	To Group 6	To Group 7
1	1.31504E-01	4.20460E-02	8.69720E-06	5.19380E-09	0.00000E+00	0.00000E+00	0.00000E+00
2	0.00000E+00	3.30403E-01	1.64630E-03	2.60060E-09	0.00000E+00	0.00000E+00	0.00000E+00
3	0.00000E+00	0.00000E+00	4.61792E-01	2.47490E-03	0.00000E+00	0.00000E+00	0.00000E+00
4	0.00000E+00	0.00000E+00	0.00000E+00	4.68021E-01	5.43300E-03	0.00000E+00	0.00000E+00
5	0.00000E+00	0.00000E+00	0.00000E+00	1.85970E-04	2.85771E-01	8.39730E-03	8.92800E-09
6	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.39160E-03	2.47614E-01	1.23220E-02
7	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.96810E-03	2.56093E-01

Table 5. Fission chamber macroscopic cross sections

	Transport	Absorption	Capture	Fission		
Group	cross section	cross section	cross section	cross section	Nu	Chi
	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )	(cm <sup>-1</sup> )		
1	1.26032E-01	5.11320E-04	5.11315E-04	4.79002E-09	2.76283E+00	5.87910E-01
2	2.93160E-01	7.58130E-05	7.58072E-05	5.82564E-09	2.46239E+00	4.11760E-01
3	2.84250E-01	3.16430E-04	3.15966E-04	4.63719E-07	2.43380E+00	3.39060E-04
4	2.81020E-01	1.16750E-03	1.16226E-03	5.24406E-06	2.43380E+00	1.17610E-07
5	3.34460E-01	3.39770E-03	3.39755E-03	1.45390E-07	2.43380E+00	0.00000E+00
6	5.65640E-01	9.18860E-03	9.18789E-03	7.14972E-07	2.43380E+00	0.00000E+00
7	1.17214E+00	2.32440E-02	2.32419E-02	2.08041E-06	2.43380E+00	0.00000E+00

Scattering block (unit: cm<sup>-1</sup>)

Group	To Group 1	To Group 2	To Group 3	To Group 4	To Group 5	To Group 6	To Group 7
1	6.61659E-02	5.90700E-02	2.83340E-04	1.46220E-06	2.06420E-08	0.00000E+00	0.00000E+00
2	0.00000E+00	2.40377E-01	5.24350E-02	2.49900E-04	1.92390E-05	2.98750E-06	4.21400E-07
3	0.00000E+00	0.00000E+00	1.83425E-01	9.22880E-02	6.93650E-03	1.07900E-03	2.05430E-04
4	0.00000E+00	0.00000E+00	0.00000E+00	7.90769E-02	1.69990E-01	2.58600E-02	4.92560E-03
5	0.00000E+00	0.00000E+00	0.00000E+00	3.73400E-05	9.97570E-02	2.06790E-01	2.44780E-02
6	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.17420E-04	3.16774E-01	2.38760E-01
7	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	4.97930E-02	1.09910E+00

Table 6. Guide tube macroscopic cross sections (unit: cm<sup>-1</sup>)

Group	Transport cross section	Absorption cross section	Capture cross section
1	1.26032E-01	5.11320E-04	5.11320E-04
2	2.93160E-01	7.58010E-05	7.58010E-05
3	2.84240E-01	3.15720E-04	3.15720E-04
4	2.80960E-01	1.15820E-03	1.15820E-03
5	3.34440E-01	3.39750E-03	3.39750E-03
6	5.65640E-01	9.18780E-03	9.18780E-03
7	1.17215E+00	2.32420E-02	2.32420E-02

Scattering block

Stattering							
Group	To Group 1	To Group 2	To Group 3	To Group 4	To Group 5	To Group 6	To Group 7
1	6.61659E-02	5.90700E-02	2.83340E-04	1.46220E-06	2.06420E-08	0.00000E+00	0.00000E+00
2	0.00000E+00	2.40377E-01	5.24350E-02	2.49900E-04	1.92390E-05	2.98750E-06	4.21400E-07
3	0.00000E+00	0.00000E+00	1.83297E-01	9.23970E-02	6.94460E-03	1.08030E-03	2.05670E-04
4	0.00000E+00	0.00000E+00	0.00000E+00	7.88511E-02	1.70140E-01	2.58810E-02	4.92970E-03
5	0.00000E+00	0.00000E+00	0.00000E+00	3.73330E-05	9.97372E-02	2.06790E-01	2.44780E-02
6	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.17260E-04	3.16765E-01	2.38770E-01
7	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	4.97920E-02	1.09912E+00

Table 7. Moderator macroscopic cross sections (unit: cm<sup>-1</sup>)

Group	Transport	Absorption	Capture
Group	cross section	cross section	cross section
1	1.59206E-01	6.01050E-04	6.01050E-04
2	4.12970E-01	1.57930E-05	1.57930E-05
3	5.90310E-01	3.37160E-04	3.37160E-04
4	5.84350E-01	1.94060E-03	1.94060E-03
5	7.18000E-01	5.74160E-03	5.74160E-03
6	1.25445E+00	1.50010E-02	1.50010E-02
7	2.65038E+00	3.72390E-02	3.72390E-02

Scattering block (unit: cm<sup>-1</sup>)

Group	To Group 1	To Group 2	To Group 3	To Group 4	To Group 5	To Group 6	To Group 7
1	4.44777E-02	1.13400E-01	7.23470E-04	3.74990E-06	5.31840E-08	0.00000E+00	0.00000E+00
2	0.00000E+00	2.82334E-01	1.29940E-01	6.23400E-04	4.80020E-05	7.44860E-06	1.04550E-06
3	0.00000E+00	0.00000E+00	3.45256E-01	2.24570E-01	1.69990E-02	2.64430E-03	5.03440E-04
4	0.00000E+00	0.00000E+00	0.00000E+00	9.10284E-02	4.15510E-01	6.37320E-02	1.21390E-02
5	0.00000E+00	0.00000E+00	0.00000E+00	7.14370E-05	1.39138E-01	5.11820E-01	6.12290E-02
6	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.21570E-03	6.99913E-01	5.37320E-01
7	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.32440E-01	2.48070E+00

Table 8. Control rod macroscopic cross sections (unit: cm<sup>-1</sup>)

Group	Transport	Absorption	Capture	
Group	cross section	cross section	cross section	
1	2.16768E-01	1.70490E-03	1.70490E-03	
2	4.80098E-01	8.36224E-03	8.36224E-03	
3	8.86369E-01	8.37901E-02	8.37901E-02	
4	9.70009E-01	3.97797E-01	3.97797E-01	
5	9.10482E-01	6.98763E-01	6.98763E-01	
6	1.13775E+00	9.29508E-01	9.29508E-01	
7	1.84048E+00	1.17836E+00	1.17836E+00	

Scattering block (unit: cm<sup>-1</sup>)

beattering	block (uliit. cii	· <i>)</i>			ı		
Group	To Group 1	To Group 2	To Group 3	To Group 4	To Group 5	To Group 6	To Group 7
1	1.7056E-01	4.4401E-02	9.8367E-05	1.2779E-07	0.0000E+00	0.0000E+00	0.0000E+00
2	0.0000E+00	4.7105E-01	6.8548E-04	3.9140E-10	0.0000E+00	0.0000E+00	0.0000E+00
3	0.0000E+00	0.0000E+00	8.0186E-01	7.2013E-04	0.0000E+00	0.0000E+00	0.0000E+00
4	0.0000E+00	0.0000E+00	0.0000E+00	5.7075E-01	1.4602E-03	0.0000E+00	0.0000E+00
5	0.0000E+00	0.0000E+00	0.0000E+00	6.5556E-05	2.0784E-01	3.8149E-03	3.6976E-09
6	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	1.0243E-03	2.0247E-01	4.7529E-03
7	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	3.5304E-03	6.5860E-01

Table 9. Delayed neutron fractions

Delayed neutron group	UO <sub>2</sub>	MOX 4.3%	MOX 7.0%	MOX 8.7%
1	2.13333E-04	7.82484E-05	7.65120E-05	7.58799E-05
2	1.04514E-03	6.40534E-04	6.34833E-04	6.33750E-04
3	6.03969E-04	2.27884E-04	2.23483E-04	2.22271E-04
4	1.33963E-03	5.78624E-04	5.68882E-04	5.66810E-04
5	2.29386E-03	9.97539E-04	9.81163E-04	9.77854E-04
6	7.05174E-04	4.33265E-04	4.29227E-04	4.29965E-04
7	6.00381E-04	3.22355E-04	3.18971E-04	3.19265E-04
8	2.07736E-04	1.23882E-04	1.21830E-04	1.21188E-04
Sum	7.00922E-03	3.40233E-03	3.35490E-03	3.34698E-03

Table 10. Delayed neutron precursor decay constants

770 77077 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
UO <sub>2</sub> , MOX 4.3%, MOX 7.0%,
MOX 8.7%
1.247E-02
2.829E-02
4.252E-02
1.330E-01
2.925E-01
6.665E-01
1.635E+00
3.555E+00

Table 11. Delayed neutron group spectra

g	1	2	3	4	5	6	7	8
				U	$O_2$			
1	0.00075	0.03049	0.00457	0.02002	0.05601	0.06098	0.10635	0.09346
2	0.98512	0.96907	0.97401	0.97271	0.93818	0.93444	0.88298	0.90260
3	0.01413	0.00044	0.02142	0.00727	0.00581	0.00458	0.01067	0.00394
4-7	0	0	0	0	0	0	0	0
				MOX	4.3%			
1	0.00075	0.03069	0.00607	0.01887	0.04990	0.05524	0.10140	0.08055
2	0.98512	0.96887	0.97276	0.97282	0.94419	0.93984	0.88508	0.91408
3	0.01413	0.00044	0.02117	0.00831	0.00591	0.00492	0.01351	0.00537
4-7	0	0	0	0	0	0	0	0

g	1	2	3	4	5	6	7	8
				MOX	7.0%			
1	0.00075	0.03069	0.00612	0.01883	0.04968	0.05506	0.10115	0.08021
2	0.98512	0.96887	0.97272	0.97283	0.94440	0.94002	0.88527	0.91438
3	0.01413	0.00044	0.02116	0.00834	0.00592	0.00492	0.01358	0.00541
4-7	0	0	0	0	0	0	0	0
				MOX	8.7%			
1	0.00075	0.03069	0.00614	0.01880	0.04960	0.05496	0.10101	0.08003
2	0.98512	0.96887	0.97270	0.97284	0.94448	0.94012	0.88540	0.91454
3	0.01413	0.00044	0.02116	0.00836	0.00592	0.00492	0.01359	0.00543
4-7	0	0	0	0	0	0	0	0

Note: each column represents one delayed neutron group (i = 1 to 8), while each row represents one of the 7 energy groups (g = 1 to 7).

Table 12. Seven-group energy structure used in preparation of cross section and kinetics parameters

	ANL structure	WIMS-D structure					
Group	Energy range (eV)	Group	Energy range (eV)				
1	1.0E+7 - 1.36E+6	1 - 4	1.0E+7 - 1.353E+6				
2	1.36E+6 - 9.2E+3	5 - 14	1.353E+6 - 9.118E+3				
3	9.2E+3 - 55.6	15 - 23	9.118E+3 - 48.052				
4	55.6 - 4.1	24 - 27	48.052 - 4.00				
5	4.1 - 0.63	28 - 45	4.00 - 0.625				
6	0.63 - 0.13	46 - 55	0.625 - 0.14				
7	0.13 - 0.0	56 - 69	0.14 - 0				

Table 13. Neutron velocities (unit: cm/s)

g	$UO_2$	MOX 4.3%	MOX 7.0%	MOX 8.7%	Moderator	Guide Tube	Fission chamber	Control rod
1	2.23466E+09	2.23473E+09	2.23479E+09	2.23483E+09	2.23517E+09	2.21473E+09	2.24885E+09	2.18553E+09
2	5.07347E+08	5.07114E+08	5.07355E+08	5.07520E+08	4.98880E+08	4.54712E+08	5.12300E+08	4.21522E+08
3	3.86595E+07	3.88385E+07	3.91436E+07	3.93259E+07	3.84974E+07	4.22099E+07	3.75477E+07	8.76487E+07
4	5.13931E+06	5.16295E+06	5.18647E+06	5.20109E+06	5.12639E+06	5.36964E+06	5.02783E+06	7.47375E+06
5	1.67734E+06	1.75719E+06	1.78072E+06	1.79321E+06	1.67542E+06	1.71422E+06	1.66563E+06	2.28533E+06
6	7.28603E+05	7.68973E+05	7.84470E+05	7.91377E+05	7.26031E+05	7.63783E+05	6.70396E+05	1.01738E+06
7	2.92902E+05	2.94764E+05	3.02310E+05	3.05435E+05	2.81629E+05	2.93629E+05	2.51392E+05	4.11374E+05

# Appendix II Original cell geometry and composition

Table 14. Pin cell geometries

Fuel cells: MOX 4.3%, MOX 7.0%, MOX8.7% and UO<sub>2</sub>

Medium	External radius (cm)
Fuel	0.4095
Void	0.4180
Zirconium Clad	0.4750
Void	0.4800
Aluminum Clad*	0.5400
Moderator (square lattice pitch)	1.26

<sup>\*</sup> This clad is used to simulate hot conditions at room temperature (decrease of the moderation ratio)

#### Guide tube cells

Medium	External radius (cm)			
Moderator	0.3400			
Aluminum Clad	0.5400			
Moderator (square lattice pitch)	1.26			

Central guide tube contains: moderator (as defined in Table 15) and 1.0E-8 at/(b·cm) of <sup>235</sup>U. In the control rod model, it is advised to directly replace the moderator with the absorber material defined in Table 16.

Table 15. Isotopic distribution for each medium (except for control rod cell)

	Table 13. Isotopic distribution for each median (except for control for each									
Nuclide			Concer	ntrations (10 <sup>24</sup> )	at/cm <sup>3</sup> )					
Nuclide	MOX 4.3%	MOX 7.0%	MOX 8.7%	$UO_2$	Moderator	Zr Clad	Al Clad			
<sup>235</sup> U	5.0000E-5	5.0000E-5	5.0000E-5	8.6500E-4						
<sup>238</sup> U	2.2100E-2	2.2100E-2	2.2100E-2	2.2250E-2						
<sup>238</sup> Pu	1.5000E-5	2.4000E-5	3.0000E-5							
<sup>239</sup> Pu	5.8000E-4	9.3000E-4	1.1600E-3							
<sup>240</sup> Pu	2.4000E-4	3.9000E-4	4.9000E-4							
<sup>241</sup> Pu	9.8000E-5	1.5200E-4	1.9000E-4							
<sup>242</sup> Pu	5.4000E-5	8.4000E-5	1.0500E-4							
<sup>241</sup> Am	1.3000E-5	2.0000E-5	2.5000E-5							
О	4.6300E-2	4.6300E-2	4.6300E-2	4.62200E-2						
$H_2O$					3.3500E-2					
B nat					2.7800E-5					
Zr nat						4.3000E-2				
<sup>27</sup> Al							6.0000E-2			

Table 16. Isotopic distribution for control rod cell

Nuclide	Concentrations (10 <sup>24</sup> at/cm <sup>3</sup> )						
	Absorber Moderator		Al cladding				
<sup>107</sup> Ag	2.27105E-2						
<sup>109</sup> Ag	2.27105E-2						
<sup>115</sup> In	8.00080E-3						
<sup>113</sup> Cd	2.72410E-3						
H <sub>2</sub> O		3.3500E-2					
B nat		2.7800E-5					
<sup>27</sup> Al			6.0000E-2				

# **Appendix III Output format**

The results of this benchmark will be presented in a benchmark report, which will be made available in both a hard copy and an electronic form. Participants are asked to provide the output information with the following requirements:

- Results will be submitted in electronic form according to templates provided by the benchmark team.
- All data should be in the units indicated in the templates (typically SI units).

The requested output for all cases will include parameters of interest defined in Section 3. Participants will be provided with an individual template file for each transient problem that includes brief introductory information and a spreadsheet for the requested output for each case. All templates will have similar format, with the following text formats:

- Black Courier New Output data to be provided by the participants,
- Blue Arial Static titles and labels that are not to be changed by participants,
- Green Arial Values automatically calculated when output is entered.

The participants are also requested to provide any information that will be helpful in explaining their results. Feedback and comments are encouraged to improve the quality and applicability of the templates. This section is only intended to provide examples of required output format and it is subject to change upon the release of finalized output templates.

#### 2-D transient

There has been a brief discussion on the parameters of interest that will be reported at each time point for the 2-D transient exercise in Section 3.1. Examples of output format are given in Table 17 for core dynamic reactivity and other integral parameters, in which the time points are shown in the first column, while the format for time dependent radial distribution of fission rate is provided in Table 18 and Table 19 on the assembly and pin basis, respectively. Note that the initial value for core reactivity and fractional total core fission rate must be 0.0 and 1.0, respectively, due to normalization requirements. In the output spreadsheet template the corresponding core dynamic multiplication factor  $k_{\text{eff}}$  (or  $k_{\text{d}}$ ) will be automatically calculated based on the input core reactivity, as shown in the 3<sup>rd</sup> column of Table 17. The definition of the effective delayed neutron fraction and prompt neutron lifetime can be found in Appendix IV.

Table 17. Exercise TD0/1/2/3 time evolution of core dynamic reactivity and fractional core fission rate

Transient	Core	Core dynamic	Fractional total	Effective	Prompt
	reactivity $\rho$	multiplication	core fission	delayed neutron	neutron
time [s]	[pcm]	factor $k_d$	rate P	fraction $\beta_{\rm eff}$	lifetime [s]
0.00	0.00000	1.00000	1.0000E+00	0.0000E+00	0.0000E+00
0.25	0.00000	1.00000	0.0000E+00	0.0000E+00	0.0000E+00
0.50	0.00000	1.00000	0.0000E+00	0.0000E+00	0.0000E+00
0.75	0.00000	1.00000	0.0000E+00	0.0000E+00	0.0000E+00
	•••	•••	•••	•••	•••
2.75	0.00000	1.00000	0.0000E+00	0.0000E+00	0.0000E+00
3.00	0.00000	1.00000	0.0000E+00	0.0000E+00	0.0000E+00
4.00	0.00000	1.00000	0.0000E+00	0.0000E+00	0.0000E+00
5.00	0.00000	1.00000	0.0000E+00	0.0000E+00	0.0000E+00
		•••		•••	•••
10.00	0.00000	1.00000	0.0000E+00	0.0000E+00	0.0000E+00

Table 18. Exercise TD0/1/2/3 radial profile of relative fission rate on assembly basis

Time [s]	0.00	
Row\Column	1	2
1	1.00E+00	1.00E+00
2	1.00E+00	1.00E+00

Table 19. Exercise TD0/1/2/3 radial profile of relative fission rate on pin basis

Time [s]	0.00				
Row\Column	1	2	3	 33	34
1	1.000E+00	1.000E+00	1.000E+00	 1.000E+00	1.000E+00
2	1.000E+00	1.000E+00	1.000E+00	 1.000E+00	1.000E+00
3	1.000E+00	1.000E+00	1.000E+00	 1.000E+00	1.000E+00
•••	•••	•••	•••	 •••	•••
33	1.000E+00	1.000E+00	1.000E+00	 1.000E+00	1.000E+00
34	1.000E+00	1.000E+00	1.000E+00	 1.000E+00	1.000E+00

# 3-D transient

The output format specified for 3-D transient problems differs from 2-D transients in asking for the 3-D map of fission rate distribution at specific time points. The C5G7 core is axially discretized into 24 planes with equal height of 5.355 cm. The node averaged fission rate is required for each axial plane at assembly and pin cell level as shown in Table 20 and Table 21, respectively, where the upper bound of each node is listed in the first column with the order from top to bottom of the core.

Table 20. Exercise TD4/5 radial profile of relative fission rate on assembly basis

	Time [s]	0.00	
Axial position [cm]	Row\Column	1	2
128.520	1	1.00E+00	1.00E+00
126.320	2	1.00E+00	1.00E+00
	1	1.00E+00	1.00E+00
•••	2	1.00E+00	1.00E+00
10.710	•••		•••
5,355	1	1.00E+00	1.00E+00
3.333	2	1.00E+00	1.00E+00

Table 21. Exercise TD4/5 radial profile of relative fission rate on pin basis

	Time [s]	0.00					
Axial position [cm]	Row\ Column	1	2	3		33	34
	1	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
	2	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
128.520	3	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
	•••	•••	•••	•••	• • •	•••	•••
	33	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
	34	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
•••	•••	•••	•••	•••		•••	•••
10.710	1	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
10./10	2	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00

	3	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
	•••	•••	•••	•••		•••	•••
	33	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
	34	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
Axial position [cm]	Row\	1	2	3		33	34
Axiai position [ciii]	Column	1	2	7	:	33	34
	1	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
	2	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
5.355	3	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
3.333		•••	•••	•••		•••	•••
	33	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00
	34	1.000E+00	1.000E+00	1.000E+00		1.000E+00	1.000E+00

## Appendix IV Additional definitions

#### Cumulative fission spectrum

The joint system of time-dependent transport equation with delayed neutrons can be written as: \*

$$\frac{1}{v} \frac{\partial \psi(w)}{\partial t} + \Omega \cdot \nabla \psi(w) + \Sigma(r, E, t) \psi(w) 
= \int \int \Sigma_{s}(r, t, \Omega', E' \to \Omega, E) \psi(w') d\Omega' dE' 
+ \tilde{\chi}_{p}(E) \int \int [1 - \beta(r, E')] v \Sigma_{f}(r, E', t) \psi(w') d\Omega' dE' 
+ \sum_{i} \tilde{\chi}_{j}(E) \lambda_{j} C_{j}(r, t)$$
(4)

and

$$\frac{\partial C_j(\mathbf{r}, \mathbf{t})}{\partial t} = -\lambda_j C_j(\mathbf{r}, t) + \int \int \beta_j(\mathbf{r}, E') \nu \Sigma_f(\mathbf{r}, E', t) \psi(\mathbf{w}') d\Omega' dE'$$
 (5)

where

$$w = \{r, \Omega, E, t\}, w = \{r, \Omega, E, t\}, \tilde{\chi} = \frac{1}{4\pi} \chi$$

In the above equations,

v = total number of neutron released per fission,

 $\chi_p(E)$  = spectrum of prompt fission neutrons,

 $\chi_j(E)$  = spectrum of the *j*-th group of delayed fission neutrons,

 $\beta_j(\mathbf{r}, E')$  = delayed neutron fraction of the *j*-th group of delayed neutrons,

 $\beta(r, E')$  = total delayed neutron fraction and  $\beta(r, E') = \sum_{i} \beta_{i}(r, E')$ ,

 $C_i(\mathbf{r}, t)$  = precursor concentration of delayed neutrons in j-th group.

For steady-state systems, the two fission terms on the right side of Eq. (4) can be combined as

$$\widetilde{\chi}_{cum}(E) \int \int v \Sigma_{f}(r, E', t) \psi(w') d\Omega' dE' 
= \widetilde{\chi}_{p}(E) \int \int [1 - \beta(r, E')] v \Sigma_{f}(r, E', t) \psi(w') d\Omega' dE' 
+ \sum_{i} \widetilde{\chi}_{j}(E) \int \int \beta_{j}(r, E') v \Sigma_{f}(r, E', t) \psi(w') d\Omega' dE'$$
(6)

where  $\chi_{cum}(E)$  is denoted as the cumulative spectrum of all fission neutrons, which represents the effective spectrum of neutron production from both direct fission and the radioactive decay of the fission product.

#### Reactivity

Define the factor F(t) as the following:

<sup>\*</sup> Bell, George I., and Samuel Glasstone. Nuclear Reactor Theory. No. TID--25606. Division of Technical Information, US Atomic Energy Commission, 1970.

$$F(t) = \int \int \tilde{\chi}_{cum}(E) \nu \Sigma_f(r, E') \psi(r, \Omega', E', t) \Phi_0^+(r, \Omega, E) dV d\Omega dE d\Omega' dE'$$
(7)

and the reactivity can be written as

$$\rho(t) = \frac{1}{F(t)} \iiint dr d\Omega dE \, \Phi_0^+(r, \Omega, E) \left\{ -\Omega \nabla \psi(r, \Omega, E, t) - \Sigma(r, E, t) \psi(r, \Omega, E, t) \right.$$

$$\left. + \iint d\Omega' dE' \left[ \Sigma_S(r, t, \Omega', E' \to \Omega, E) \right. \right.$$

$$\left. + \tilde{\chi}_{cum}(E) \nu \Sigma_f(r, E', t) \right] \psi(r, \Omega', E', t) \right\}$$

$$(8)$$

where  $\Phi_0^+$  is the adjoint function, which is defined as the fundamental mode eigenfunction of the equation adjoint to the time independent transport equation.

# Effective delayed neutron fraction

Similarly, the effective delayed neutron fraction of j-th group has the following expression:

$$\beta_{j}(t) = \frac{1}{F(t)} \int \dots \int \tilde{\chi}_{j}(E) \beta_{j} \nu \Sigma_{f}(r, E', t) \psi(r, \Omega', E', t) \Phi_{0}^{+}(r, \Omega, E) dV d\Omega dE d\Omega' dE'$$
(9)

The total effective delayed neutron fraction is nothing but the summation of all delayed neutron groups:

$$\bar{\beta}(t) = \sum_{j} \bar{\beta}_{j}(t) \tag{10}$$

#### Prompt neutron lifetime

The prompt neutron lifetime as a function of time can be written as

$$\Lambda(t) = \frac{1}{F(t)} \int \dots \int \frac{1}{v} \psi(r, \Omega, E, t) \Phi_0^+(r, \Omega, E) dV d\Omega dE$$
 (11)