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Preliminary Results for the OECD/NEA Time Dependent Benchmark using Rattlesnake, Rattlesnake-IQS and TDKENO

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1 Introduction

The Transient Reactor Test Facility (TREAT) is an air-cooled, thermal-spectrum test facility designed to evaluate reactor fuels and structural materials under simulated nuclear excursions and transient power/cooling mismatch situations in a nuclear reactor [2]. The U.S. Department of Energy Office of Nuclear Energy (DOE/NE) is preparing to resume operation of TREAT, which is located at Idaho National Laboratory (INL), by 2018 [3].

The INL is currently evolving the modeling and simulation (M&S) capability that will enable improved core operation as well as design and analysis of TREAT experiments. This M&S capability primarily uses MAMMOTH [4], a reactor physics application being developed under the Multi-physics Object Oriented Simulation Environment (MOOSE) framework [5]. MAMMOTH allows the coupling of a number of other MOOSE-based applications.

One goal of the MAMMOTH M&S project is to validate the analysis capabilities within MAMMOTH. Historical data has shown limited value for validation of full three-dimensional (3D) multi-physics methods[6]. Initial analysis considered the TREAT startup minimum critical core[7] and one of the startup transient tests[8]. At present, validation is focusing on measurements taken during the M8CAL test calibration series[9]. These exercises will valuable in preliminary assessment of the ability of MAMMOTH to perform coupled multiphysics calculations; calculations performed to date are being used to validate the neutron transport solver Rattlesnake[10] and the fuels performance code BISON[11].

However, other validation projects outside of TREAT are available for single-physics benchmarking. Because the transient solution capability of Rattlesnake is one of the key attributes that makes it unique for TREAT transient simulations, validation of the transient solution of Rattlesnake using other time dependent kinetics benchmarks has considerable value. The Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD) has recently developed a computational benchmark for transient simulations[1]. This benchmark considered both two-dimensional (2D) and 3D configurations for a total number of 26 different transients. All are negative reactivity insertions, typically returning to the critical state after some time. The benchmark specification is included as Appendix A.

This benchmark, when complete, will consist of submissions from a number of code systems and from a collection of international participants. As such, it should provide a fair comparison of existing analysis methods. It is unlikely that the benchmark will be com-

pleted and published for at least two years, but it does provide a set of tests that can be used to compare Rattlesnake's implicit time dependent solution, the recently implemented Improved Quasi-Static (IQS) approximation within Rattlesnake[12], and the time-dependent Monte-Carlo-based solver TDKENO[13].

This report summarizes the status of a work in progress. The benchmark specification itself remains somewhat fluid as ambiguities remain. The set up of the cases has allowed identification of some of these ambiguities, and the benchmark team has been made aware of these issues. But our purpose here has been to use the benchmark to compare implicit and IQS solutions, and to use the TDKENO solutions as a point of comparison.

2 Benchmark Overview

The full details of the C5G7-TD benchmark are provided in Appendix A. This section provides a quick overview of the benchmark configuration and the various exercises within the benchmark. The benchmark, often referred to as the C5G7-TD (time dependent) benchmark, is based on the configuration from the earlier C5G7 MOX benchmark[14]. That benchmark was a steady-state simplified quarter-core configuration containing two MOX and two UO_2 fuel assemblies. This benchmark was selected for this work simply because it was a small core, discrete pin model with control rods for which many participants could resurrect as a starting point for this benchmark. The axial dimensions on the original benchmark were extended somewhat for this study. The core has a water reflector axially and radially, with control rods initially present in the top reflector area, extended to the top of the core. The core cofiguration is shown schematically in Fig. 2. Both UO_2 and MOX assemblies are based on the Westinghouse 1717 configuration, consisting of 264 fuel pins, 24 guide tubes for control rods and one instrument tube for a fission chamber in the center cell location, as shown in Fig. **??**. All pin cells have a pin radius of 0.54 cm with a pitch of 1.26 cm; the clad and fuel are homogenized. The MOX assemblies have three enrichments of 4.3%, 7.0%, and 8.7%., The two UO_2 assemblies are uniformly loaded with 3.7% enriched uranium.

The benchmark is divided into 6 exercises, TD0 - TD5. Table 1 provides a brief description of each exercise. Within each exercise, variations are made in the control rod banks inserted (one bank for each of the four assemblies in the quarter-core model), or in the moderator density. TD0 uses step insertions and removals of reactivity, while the other exercises use linear insertion and removal of reactivity.

For the 2D models, rod insertion was simulated by time-dependent mixing of the water/tube cross-sections and the control rod cross sections, i.e., for a 1% rod insertion, the guide tube region goes from using guide tube cross sections to 0.99guide tube cross sections + 0.01control rod cross sections.

The specification is comprized of 8 unique materials: three MOX enrichments, UO_2, guide tube (homgenized with interior water), instrument tube (homogenized with fission chamber), control rod and water. Seven energy group cross sections are provided for each material with P0 scattering, along with neutron kinetics data for eight delayed neutron groups.

The remainder of this report describes the approach taken in performing calculation. Section 3 describes the standard Rattlesnake direct or implicit time step approach, and provides

Table 1: Benchmark Exercise Descriptions

Exercise ID	2D/3D	Number of Problems	Description
TD0	2D	5	Step insertion of 10% of rod length, followed by step removal of 5%, another 5% later.
TD1	2D	5	Linear insertion of 1% of rod length, followed by linear removal of full 1% of rod.
TD2	2D	3	Linear insertion of 10% of rod length, followed by linear removal of full 10% of rod.
TD3	2D	4	Linear decrease of water density, followed by linear increase to original density. 10% of rod.
TD4	3D	5	Linear insertion of 33% of rod length, followed by linear removal of full 33% of rod.
TD5	3D	4	Linear decrease in water density, varying by location, followed by return to original density.

the results of a number of calculations. Section 4 describes the IQS approach recently implemented in Rattlesnake[12] and compares results from those calculations to those of the direct solutions. Finally, Section 5 describes the approach taken and results of TDKENO calculations for those problems that have been completed. Section 6 will describe findings of these comparisons.

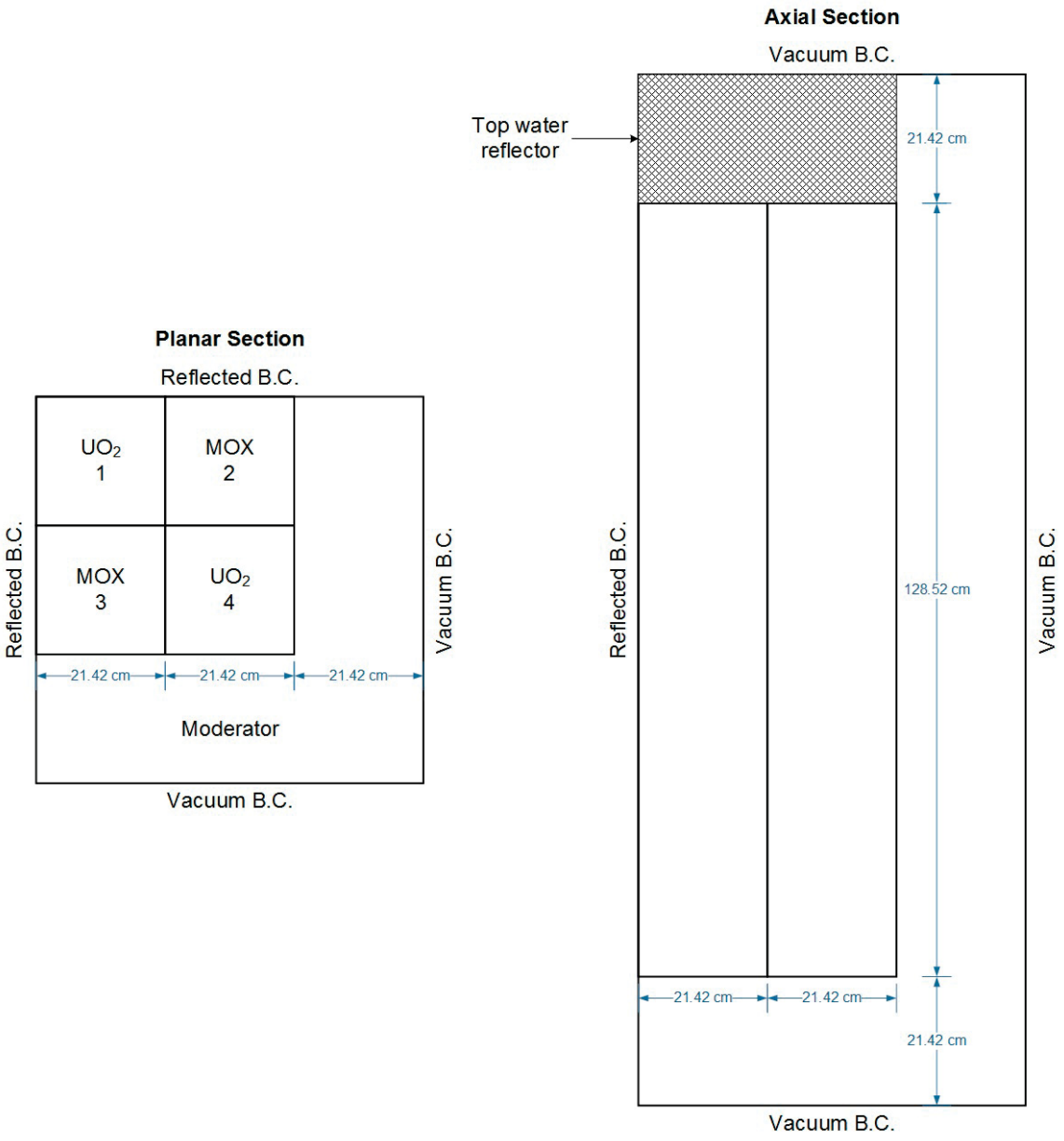

Figure 1: 3-D configuration for the C5G7-TD benchmark problem[1]

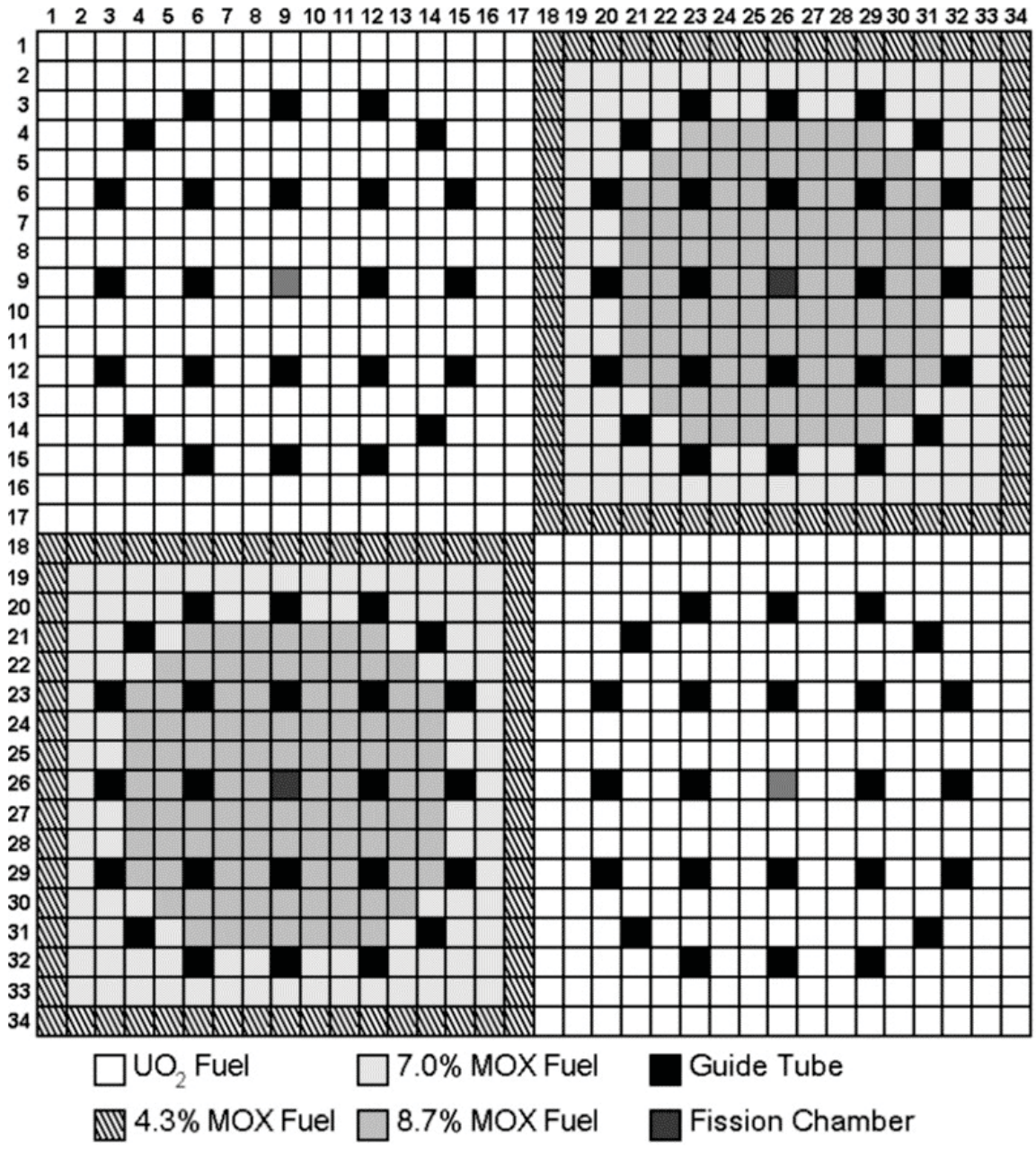

Figure 2: C5G7-TD benchmark fuel pin compositions and numbering scheme[1]

3 Rattlesnake Implicit Calculations

Rattlesnake requires a finite element mesh for which the calculation is to be performed. Often generation of a mesh is the most difficult process for reactor modeling. Fortunately, the INSTANT package[15], a predessor to Rattlesnake, is able to automatically generate 2D meshes for LWR-type configurations. The INSTANT mesh generator is available within a MAMMOTH build structure, e.g. */projects/mammoth/yak/contrib/instant/instant_mesh_generator-opt*. The input for instant_mesh_generator-opt is an XML specification. The XML file used to create the C5G7 mesh is provided in Appendix B. The result of the mesh generation process is an Exodus[16] format file. In this case, file *c5g7-td-2d-base.e*. This mesh was used for exercises TD0-TD3.

Exercises TD4 and TD5 are 3D benchmarks based on the 2D mesh. In this case, it is easy to use the mesh extruder available within Rattlesnake through the libMesh package included within MOOSE. This is accomplished by running Rattlesnake with a

mesh-only flag, e.g., */projects/mammoth /rattlesnake/rattlesnake-opt -i c5g7-td-3DExtrusion.i -mesh-only*. Part of the extrusion process allows for redefining material blocks. Hence, per the specification, the bottom 21.42 cm of the mesh were all assigned to the water reflector material block. The top 21.42 cm were assigned water outside the guide tube locations, with control rod material in place of guide tube materials. Unique control rod blocks were used for each of the four different assemblies, so that the blocks can be modified independently. The input to perform these operations is provided in Appendix C.

The Rattlesnake solution for a transient calculation is performed at two calculations: (1) the initial eigenvalue solution, and (2) the fixed source transient calculation, which starts with the fluxes from the eigenvalue solution. The MOOSE *MultiApp and Transfer* system was used to link the two calculations. Two inputs are therefore required, one for the transient and one for the initial stead state calculation. The meshes and energy structures are required to be the same for a simple transfer. The MultiApp and Transfer input section from the transient calculations is provided below:

```
[MultiApps]
 [./initial_solve]
   type = FullSolveMultiApp
```

```
   execute_on = initial
   input_files = c5g7-td_initial.i
 [../]
[]

[Transfers]
 [./copy_solution]
   type = TransportSystemVariableTransfer
   from_transport_system = diffusion
   to_transport_system = diffusion
   direction = from_multiapp
   multi_app = initial_solve
   execute_on = initial
 [../]
[]
```

In short, this block tells Rattlesnake to run case textitc5g7-td_initial.i] before starting this calculation, then transfer the solution from that calculation to me so I can start from there. Because the initial conditions and meshes are identical for all of the two dimensional cases, these two blocks of input are identical in those cases. Hence, only a single 2D input is required. The steady state input *c5g7-td_initial.i* is provided in Appendix D. Note that the 3D cases work on the same principle, and all share a single initial input. That input is essentially the same as is used for 2D, but points to a 3D mesh, and has additional material assignments for the new material blocks in the 3D extrusion.

Seven energy group cross sections and data for eight delayed neutron groups are provided in the benchmark. However, for both the 2D and 3D cores thes cross sections yield a supercritical core. Because kinetics calculations assume a reactor in initially critical before perturbations are applied, it is necessary to modify the cross sections to get a critical system. The benchmark specification suggests modification of either ν or σ_f. In the Rattlesnake XML cross section file, ν is not provided; rather the combined term $\nu\sigma_f$ is used. Hence, this term was divided by the eigenvalue computed for the provided cross sections. Different eigenvalues are computed for the 2D and 3D cases; k_{eff} = 1.1839374620 was calculated for the 2D problem, while a k_{eff} value of 1.1624310525 was calculated for the 3D core. Hence, the original cross sections were modified to create one set for 2D calculations and another for 3D calculations.

At this time the 3D problems are incomplete - the initial steady state calculation has been tested and result look reasonable, but the transient calculations have not been completed. For the 2D calculations, exercises TD0-TD2 use 2D-simulated rod insertions; TD3 uses moderator decreases to decrease reactivity. All transients use essentially the same inputs, although rod motions are simulated in the 3D cases while concentration of control rod is added to the guide tube mixure. A sample input for the TD0.1 case is provided in Appendix E.

The TD0 exercise consists of an instanteous insertion of a 10% of control rod bank(s) at time zero, withdrawal to 5% at 1 second, then full withdrawal at 2 seconds. The calculations are performed for different sets of rod banks, where the rod bank number corresponds to the assembly number, as given in Fig. 1. The five cases in this exercise are as follows:

- 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.

```
[Functions]
  [./rodMove]
#  TD0
      type = StepFunction
      timep = '0.0 1.0 2.0'
      value = '0.0 0.01 0.005 0.0'
  [../]
[]
```

This function simply returns a fraction as a function of time based on the step function specification. For each control rod bank to be moved in a calculation, the material specification for a time dependent control rod was provided inside the input `[Materials]` block:

```
[./GuideTube_Z1]
    type = CRoddedNeutronicsMaterial
    block = 'M-15-TRI'
```

```
    position_as_fraction = true
    material_ids = '8 5'
    front_position_function = rodMove
[../]
```

This specification tell the code to mix the control rod material (8, the first ID) with the follower (5, guide tube material), as a fraction, as specified by $front_position_function$. This function is *rodMove* as described above. For other banks, the standard neutronics material assignment was used:

```
[./GuideTube_Z2]
    type = ConstantNeutronicsMaterial
    block = 'M-25-TRI'
    material_id = 5
[../]
```

In this excerpt the mesh block (25) for assembly no. 2 guide tube positions is assigned to material 5. In performing these calculation the rod motion functions were assigned to the bank(s) being moved, while the other banks were set as *ConstantNeutronicsMaterial*.

Figure 3 shows the results of the five calculations. The form of the transients is consistent with expectations. Bank 1, located at the center of the core, is seen to have much more worth than the other banks; banks 3 and 4 are on the border with the reflector, and have less reactivity worth. Prompt drop and prompt jump responses are see, with magnitudes corresponding to the worth of each bank or set of banks. Delayed neutron effects are seen after each rod movement.

The TD1 exercise uses linear rod insertion, to a max of 1%. Rod insertion begins at zero insertion, reaches 1% at 1 second, then is linearly drawn out to be fully withdrawn by 2 seconds. This exercise uses the same 5 cases as were used in TD0. The results of the five TD1 calculations are provided in Fig. 4. The shape of the curves show the expected form for a linear insertion and withdrawal, and the magnitude of the different cases for different bank operations is consistent with TD0.

For this case, inputs are the same as were used in the TD0 exercise, with the exception of the *rodMove* function. The form of the function is changed from

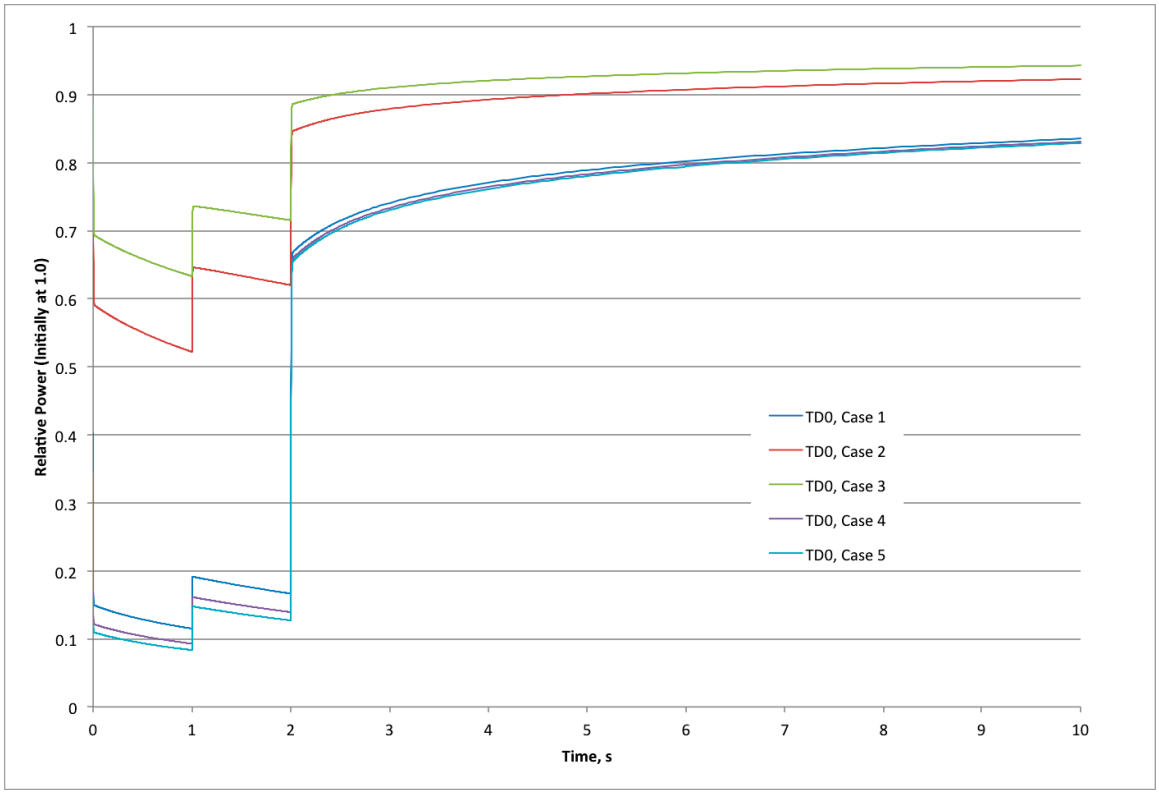

Figure 3: Results of Exercise TD0, direct solution.

a *StepFunction* to a *SlopeFunction*. The SlopeFunction is used to linearly interpolate between values for each time step. In this calculation, the maximum insertion was changed from 10% of TD0 to 1%. In this case, the four bank insertion power drops to approximately 50% of the initial value.

```
[Functions]
  [./rodMove]
#  TD1
    type = SlopeFunction
    timep = '0.0 1.0 2.0 10.0'
    value = '0.0 0.01 0.0 0.0'
  [../]
[]
```

The third exercise, TD2, is a duplication of TD1, with the exception that the

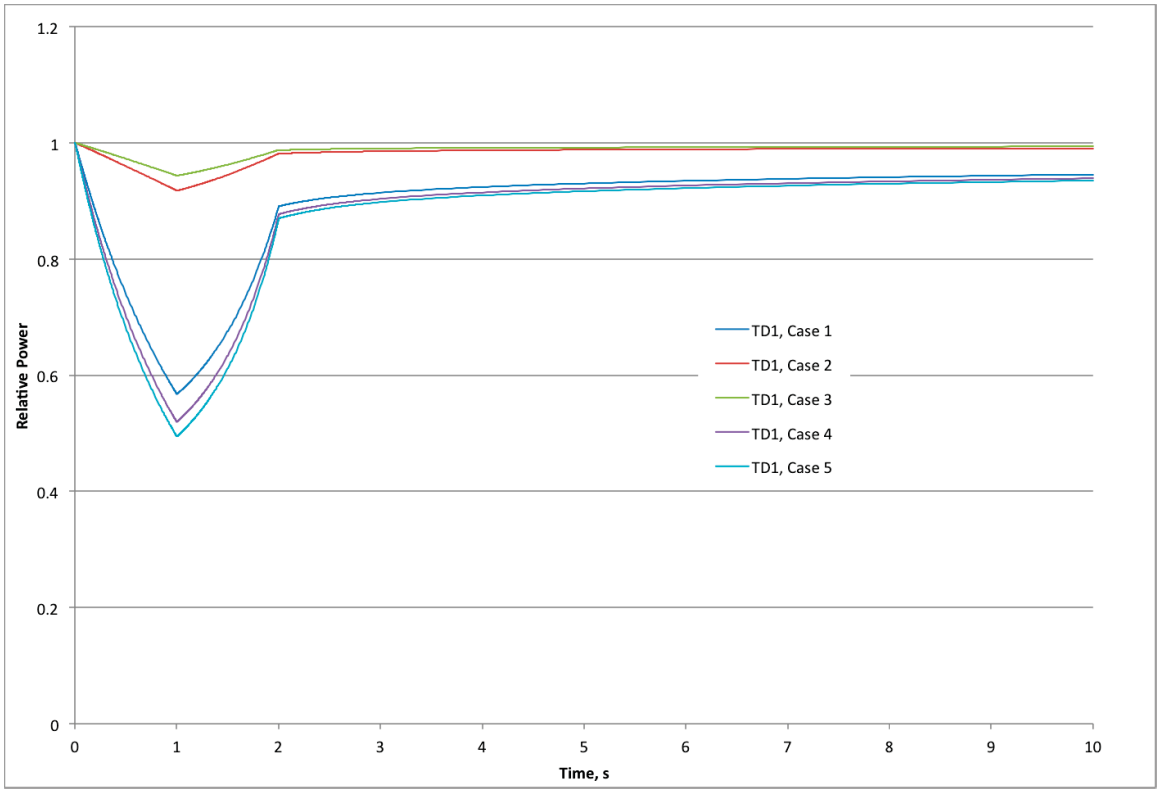

Figure 4: Results of Exercise TD1, direct solution.

control rod is inserted to 10% rather that 1% over the same time period, then withdrawn over the same period. For this exercise, only three transient calculations are requested:

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

The results of these calculations are illustrated in Fig. 5. As one would expect, the shape of the power curve during rod movement is similar to that of exercise TD1, and the magnitude is significantly larger.

Exercise TD3 uses water density changes instead of rod motion. 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

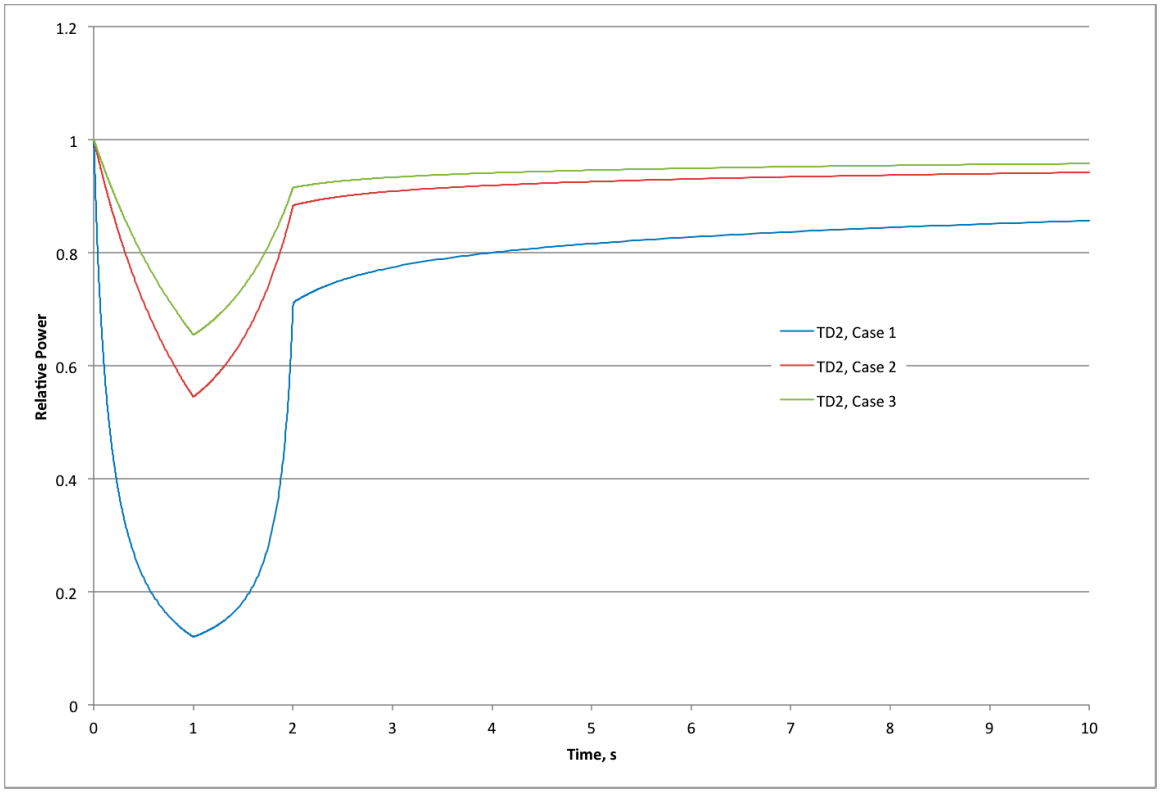

Figure 5: Results of Exercise TD2, direct solution.

s into the transient. This minimum value is represented as a fraction, denoted as ω ($0 \leq \omega \leq 1$), of its initial value. The moderator density then linearly returns to its initial value within next 1 s. Four cases were run, with varying values of ω:

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

Because the *rodMove* function used earlier was used to homogenize control rod and guide tube cross sections by fraction, the same approach can be used to change the water density. A new water material, ID 17, was created with all cross sections reduced to 80% of the nominal water cross sections. Mixing

fractions of 0.25, 0.50, 0.75, 1.00 were used to to obtain 0.95, 0.90, 0.85 and 0.80 values for rho. The function name *rodMove* was changed to *densChange* for readability - the original name could have been used.

```
[Functions]
  [./densChange]
#TD3
    type = SlopeFunction
    timep = '0.0 1.0 2.0 10.0'
    value = '0.0 0.25 0.0 0.0'
  [../]
[]
```

For this exercise the water density change was applied only to the moderator, i.e., the water within the fuel assemblies. The reflector, the water outside the fuel assemblies, was maintained at the original density through the transient. Hence, a new block, M-17-TRI, was created to distinguish between moderator and reflector. The moderator was then defined as:

```
  [./moderator]
    type = CRoddedNeutronicsMaterial
    block = 'M-7-TRI'
    position_as_fraction = true
    material_ids = '17 7'
    front_position_function = densChange
  [../]
```

and the reflector is maintained at a constant density:

```
  [./reflector]
    type = ConstantNeutronicsMaterial
    block = 'M-17-TRI'
    material_id = 7
  [../]
```

The results of this calcuation are shown in Fig. 6. Because the reactivity is changed linearly, the general shape of the power transient matches the form of

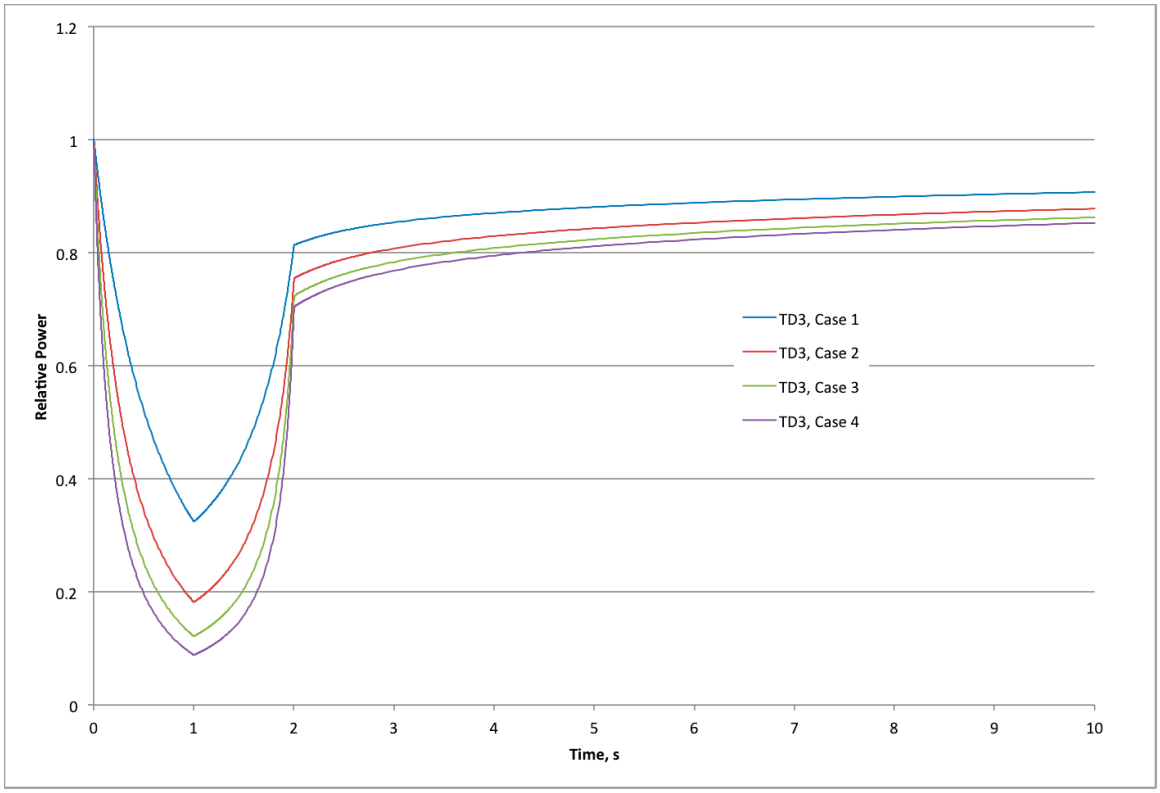

Figure 6: Results of Exercise TD3, direct solution.

TD1 and TD2 results. Not surprisingly, the power minimum, corresponding to the largest reactivity change, occurs with $\omega = 0.80$.

As discussed earlier, the 3D TD4 exercise is still in progress. Because it is a 3D case, the rod insertion is modeled directly as an insertion. Control rods start at the interface between the top of the core and the upper reflector region, and move in a downward Z direction. The input logic for this motion is as follows. First, the material specification for the moving control rod bank is:

```
[./GuideTube_Z1]
  type = CRoddedNeutronicsMaterial
  block = 'M-15-TRI'
  material_ids = '8 5 5'
  rod_withdrawn_direction = z
  front_position_function = rodMove
[../]
```

The *rodMove* function is changed to describe a physical control rod movement from the top of the core to the specified insertion position:

```
[Functions]
  [./rodMove]
#  TD4
    type = SlopeFunction
    timep = '0.0 2.1 4.1 10.0'
    value = '149.9 107.1 149.9 149.9'
  [../]
[]
```

As indicated earlier, this calculation is still in progress. The current results (for case TD4.1, with rods 33% inserted) are shown in Fig. 7. The prompt drop seen at the very beginning of the insertion is not expected; the behavior should be similar to that seen in the previous 2D transients with linear insertion/withdrawal. Additionally, there are "wiggles" in the curve, rather that the expected smooth curve before and after the peak solution. It is believed that this is due to the discretized axial model used for the 3D core - a new mesh with a finer axial mesh is needed.

All of the solutions completed so far are for the implicit solution of the time-dependant transport equation coupled with eight delayed neutron equations. Recent work within Rattlesnake has added an "Improved Quasi-Static" or IQS approach for acceleration of the time-dependent solution. The following section describes inital IQS calculations for these benchmarks, and compares to the implicit solution.

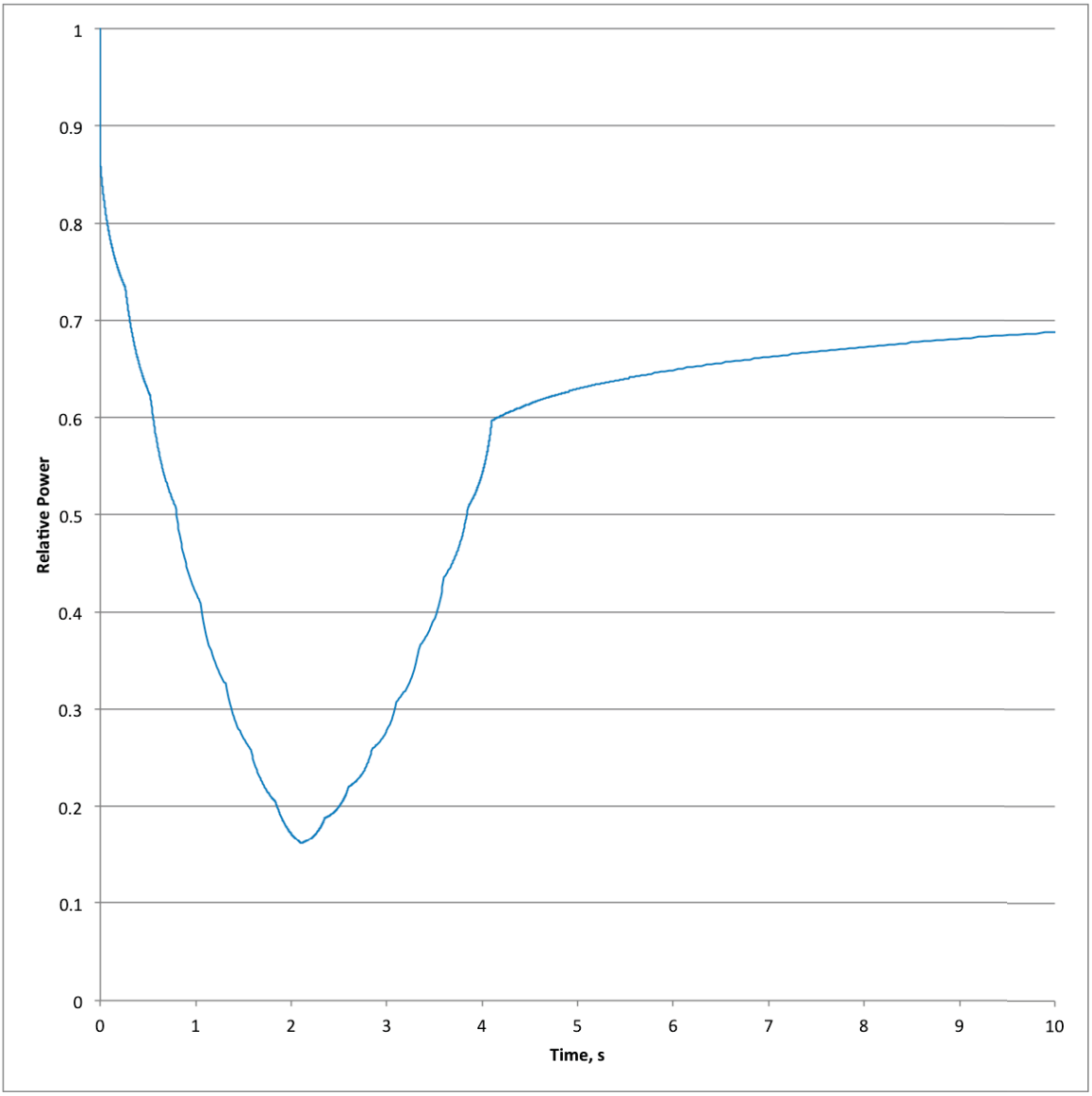

Figure 7: Curent results of Exercise TD4 Case 1, direct solution.

4 Rattlesnake IQS Calculations

The improved quasi-static (IQS) method is a transient spatial kinetics method that involves factorizing the neutron flux into a space- and time-dependent component (the shape) and a time-dependent component (the amplitude) [17, 18]. The technique relies on the shape being less rapidly varying in time compared to the flux, hence requiring fewer shape computations or updates. The IQS method has primarily been developed in the context of the neutron diffusion approximation [19, 20], but reference [21] provides an extension of the technique to transport, implemented in TDTORT and TDKEO. This section includes a brief description of IQS and how it works in Rattlesnake.

IQS evaluates two coupled systems of equations: a shape-diffusion equation and a point reactor kinetics equation (PRKE). The shape-diffusion equation is very similar to a full flux-diffusion described in the previous section, but the shape's volume integrated quantity is constant. The PRKE is a zero-dimensional amplitude evaluation, which computes essentially instantaneously compared to diffusion evaluations of complex geometries. And the constant integral quantity of the shape makes it weakly dependent on time with symmetric reactivity perturbations in a reactor geometry. Therefore, the PRKE can can be solved on much finer time scale (micro time steps) than the shape (macro time steps) while retaining accuracy; this saves an exceptional amount of computation time compared to typical implicit calculations. Figure 8 shows a time-scale visualization of the IQS process.

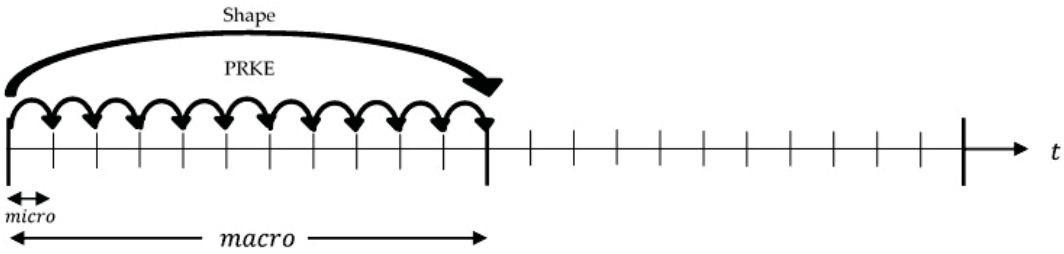

Figure 8: IQS method visualization

Rattlesnake implements two different versions of IQS: traditional IQS and IQS predictor-corrector (IQS P-C). Since only IQS P-C was applied to the benchmark, this report will only describe the IQS P-C technique. Rattlesnake first performs a full diffusion evaluation on the macro step scale to obtain a pre-

dicted flux. Using this flux, post-processors and user-objects compute the flux-dependent parameters of the PRKE. Using an interpolation of these parameters, the PRKE evaluated on the micro step time scale to obtain a amplitude at the end of the macro step. The predicted flux is then scaled by the amplitude to obtain a corrected flux.

For IQS P-C (referred to hereafter as simply IQS), the input structure in somewhat different. For IQS calculations, both forward and adjoint solutions are required. The IQS solver within Rattlesnake is aware of this and expects to see fluxes from each solution. The MultiApp/Transfer system is used to run both calculations and automatically transfer information.

```
[MultiApps]
 [./initial_solve]
   type = FullSolveMultiApp
   execute_on = initial
   input_files = c5g7-td-IQS_initial.i
 [../]
 [./adjoint_solve]
   type = FullSolveMultiApp
   execute_on = initial
   input_files = c5g7-td_adjoint.i
 [../]
[]

[Transfers]
 [./copy_solution]
   type = TransportSystemVariableTransfer
   from_transport_system = diffusion
   to_transport_system = diffusion
   direction = from_multiapp
   multi_app = initial_solve
   execute_on = initial
 [../]
 [./copy_adjoint]
   type = MultiAppVariableTransfer
   execute_on = initial
   direction = from_multiapp
   multi_app = adjoint_solve
```

```
   from_variables = 'sflux_g0 sflux_g1 sflux_g2 sflux_g3 sflux_g4 sflux_g5 sflux_
   to_variables = 'adjoint_flux_g0 adjoint_flux_g1 adjoint_flux_g2 adjoint_flux_g
 [../]
[]
```

As with the implicit solution these operations are the same for all IQS cases and thus are in all IQS inputs.

The executioner block has a few differences too. The IQS executioner is shown below. Differences are the variables *numsteps*, which defines the number of time steps taken for the transport solution; *nmicro*, which is the number of point kinects calculations run between transport solutions; *predictor_corrector*, which tells Rattlesnake whether or not to use the IQS predictor-corrector code; *prke_scheme*, which defines the time discretization scheme to use in the IQS kinetics solve; and *pke_param_csv*, which tells Rattlesnake to output point kinects solution as a comma separated variable file, using the fine name provided.

```
[Executioner]
   type = IQS
   predictor_corrector = true
   pke_param_csv = c5g7-td_IQS_0.1_params.csv

   start_time = 0.0
   end_time = 10
   num_steps = 1000
   n_micro = 10000
   prke_scheme = 'RK'
   l_tol = 1e-2
   nl_max_its = 200
   nl_rel_tol = 1e-6
   nl_abs_tol = 1e-8

   solve_type = 'PJFNK'
   petsc_options_iname = '-pc_type -pc_hypre_type -ksp_gmres_restart '
   petsc_options_value = 'hypre boomeramg 100'
[]
```

For the TD0 cases, 1000 transport solutions were required to be able to catch the effect of the instaneous rod movement (step insertion); other cases with

linear insertion only required 100 (and perhaps fewer) transport solutions. Ideally one would use small time steps only in the vicinity of the step change. However, IQS is not currently compatible with existing schemes for variable timestep sizes as a function of time. Such a capability has been developed but has not been reviewed and pushed into the main repository branch, so is not yet available to standard users.

The results of the IQS calculations for Exercise TD0 are shown in Fig. 9. One can see that these result are very close to the implicit solution results show earlier (see Fig. 3). Results can't be compared in a relative difference sense as the two calculations do not use the same time steps, so there are no 1:1 comparison points. That will be addressed in later studies. However, Fig. 10 shows implicit and IQS results plotted together for cases 1 and 2; the results are essentially identical from the two methods. This demonstrates that the IQS approximation is a very accurate approximation to a direct solution of the transport equation.

Figures 11 and 12 show the results for the TD1 Exercise, and again demonstrate that the IQS solution is in extremely good agreement with the direct solution. For these calculations, the number of transport time steps was reduced from 1000 to 100. The direct solutions required on the order of 1000 time steps - the IQS solution shows extremely good agreement to those solutions with an order of magnitude fewer transport solutions.

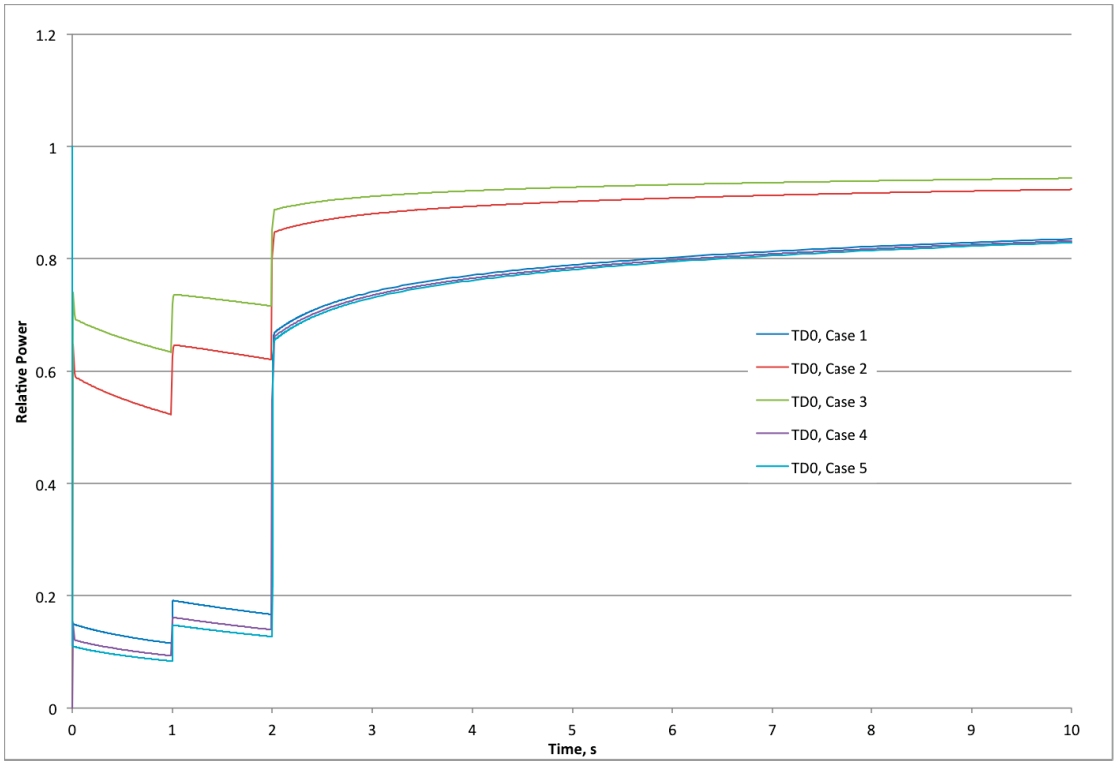

Figure 9: Results of Exercise TD0, IQS solution.

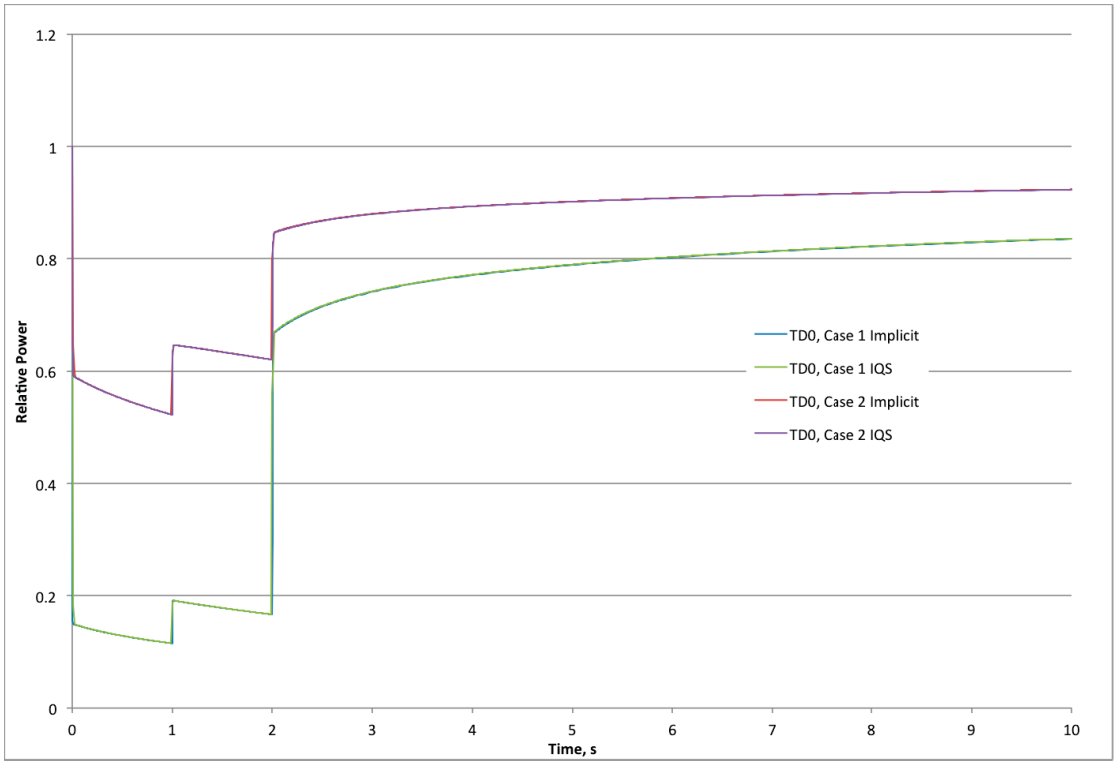

Figure 10: Comparison of selected Exercise TD0 results, IQS solution vs Direct Solution.

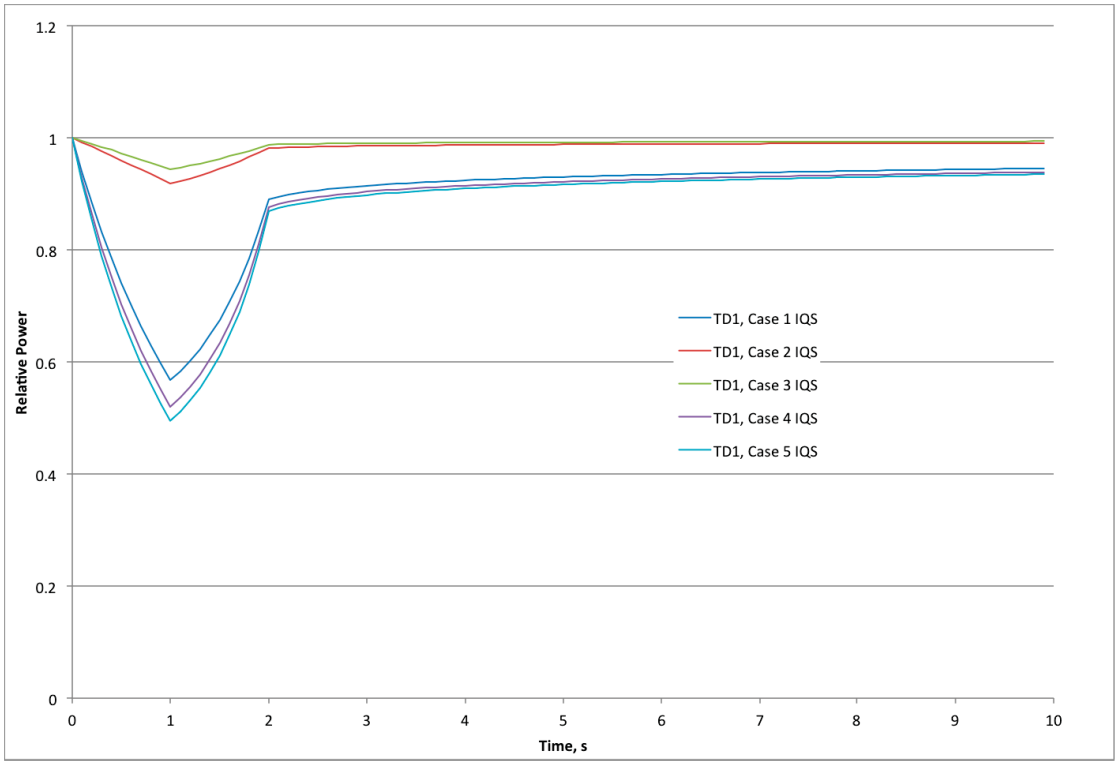

Figure 11: Results of Exercise TD1, IQS solution.

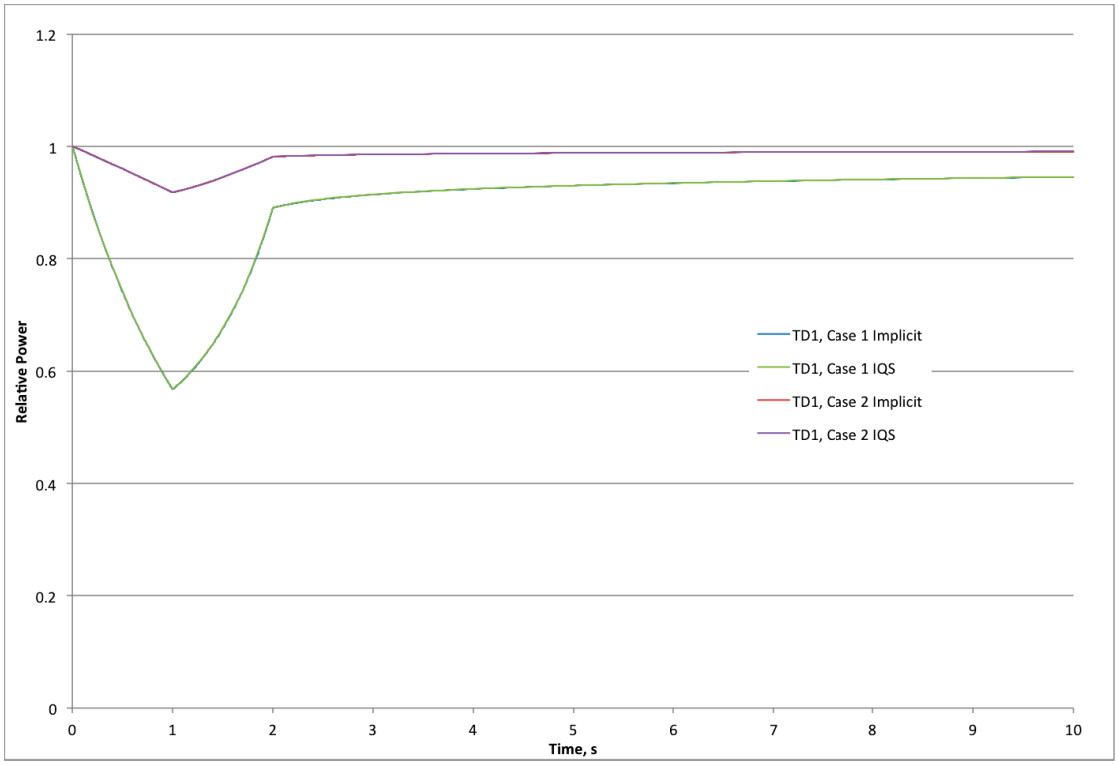

Figure 12: Comparison of selected Exercise TD1 results, IQS solution vs Direct Solution.

5 TDKENO Calculations

Students and faculty at the University of Florida (UF) have been supporting efforts for evaluating the kinetics capabilities of Rattlesnake by using TDKENO to provide an independent comparison to TREAT simulations using Rattlesnake without feedback. They are also participating in this benchmark and communicating results with INL staff.

TDKENO is a computer program that uses a hybrid method for solving the time-dependent, three dimensional (3-D) Boltzmann transport equation with explicit representation of delayed neutrons [13], [22], [23]. TDKENO utilizes the IQS method, which is a flux factorization method[24]. In flux factorization methods, the flux is assumed to be factored into a purely time-dependent amplitude function which varies quickly with time and a flux shape function which varies slowly with time. This relationship can be explicitly represented as seen in Equation (1) where (r,E,,t) is the angular flux at position r, energy E and time t; T(t) is the amplitude function and (r,E,,t) is the flux shape function with weak time dependence.

$$\Psi(r,E,\Omega,t) = T(t)\,.\,\phi(r,E,\Omega,t)$$

The position, energy, and angle dependent neutron flux shape is computed using modified versions of the well-known 3-D Monte Carlo codes KENO V.a [25] or KENO-VI [26]. Solving the shape equation, which is a modified form of the 3-D transport equation, is computationally expensive. However, by taking advantage of the parallel computation capabilities of KENO, computation of shape function is sped up. The flux shape calculated by KENO is used to compute the point kinetics parameters (e.g., reactivity, generation time, effective delayed neutron fractions, etc.). Rapidly varying amplitude equation is solved deterministically many times between shape calculations to obtain a highly accurate solution without the expense of direct integration. TDKENO is a hybrid analysis tool due to use of both a stochastic (KENO computing the flux shape) and deterministic (solving the point kinetics equations) method for determining a solution.

The initial step in a given problem is to perform a steady state adjoint calculation using KENO. Note that this can be turned off if the adjoint flux is already known and provided in the working directory. The steady state adjoint flux is used as a weighting function in the IQS method in calculating the point kinet-

ics parameters. Similarly, the forward calculation is done with KENO to determine the initial flux shape, the effective multiplication factor, and constraint integral. Prior to running TDKENO for a transient analysis, the user needs to prepare multigroup cross section libraries that correspond to the initial state of the system as well as all perturbed states. Perturbation is realized by replacing the actual cross section values for a given material in the cross section library without changing the material number. The cross section files are created by running a KENO calculation with the materials corresponding to that state and saving the KENO-generated Monte Carlo-formatted cross section library. If the cross sections are provided as a text file, one can use the newly developed cross section generation tool to create an AMPX-formatted cross section library for use in TDKENO. TDKENO linearly interpolates between the user provided cross section sets to determine the system cross sections at each reactivity time step while solving for the amplitude function. However, KENO itself only uses the user-provided cross section files to compute the flux shape, i.e., no new cross section file is created as a result of internal interpolation. Therefore the user must provide the cross section files in such a manner that using those files with KENO and linear interpolation inside TDKENO would result in correct representation of the system cross sections at all times.

Thus far UF has completed the TD0 set of calculations. Differences were observed between TDKENO and Rattlesnake results, and current efforts are focused on identifying the reason for the differences before moving on to the TD1 exercises. Figure 13 shows the results of TDKENO calculations for the TD0 Exercise; viewed by itself these results appear consistent with the Rattlesnake results in the previous two sections. However, when compared directly, differences are seen in the power decrease during the initial prompt drop, and again for the prompt jump after insertion. Figures 14 - 18 show TDKENO results compared to Rattlesnake results for each of the five cases in TD0. Interestingly, good agreement is seen for Case 2 (Fig. 15), but the other cases underpredict the prompt drop relative to Rattlesnake at time zero. It appears that the prompt jump has a corresponding overprediction, such that the solutions are in relatively good agreement after two seconds into the transient. INL is working closely with UF to resolve the differences.

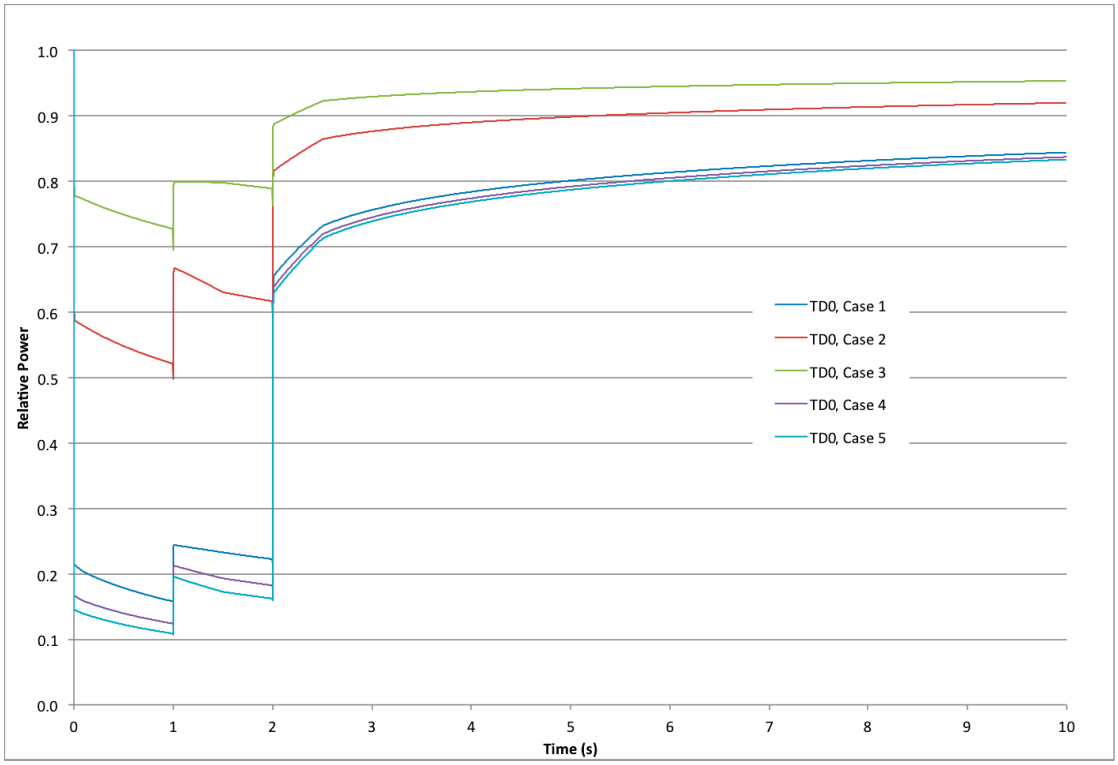

Figure 13: Results of Exercise TD0, TDKENO solution.

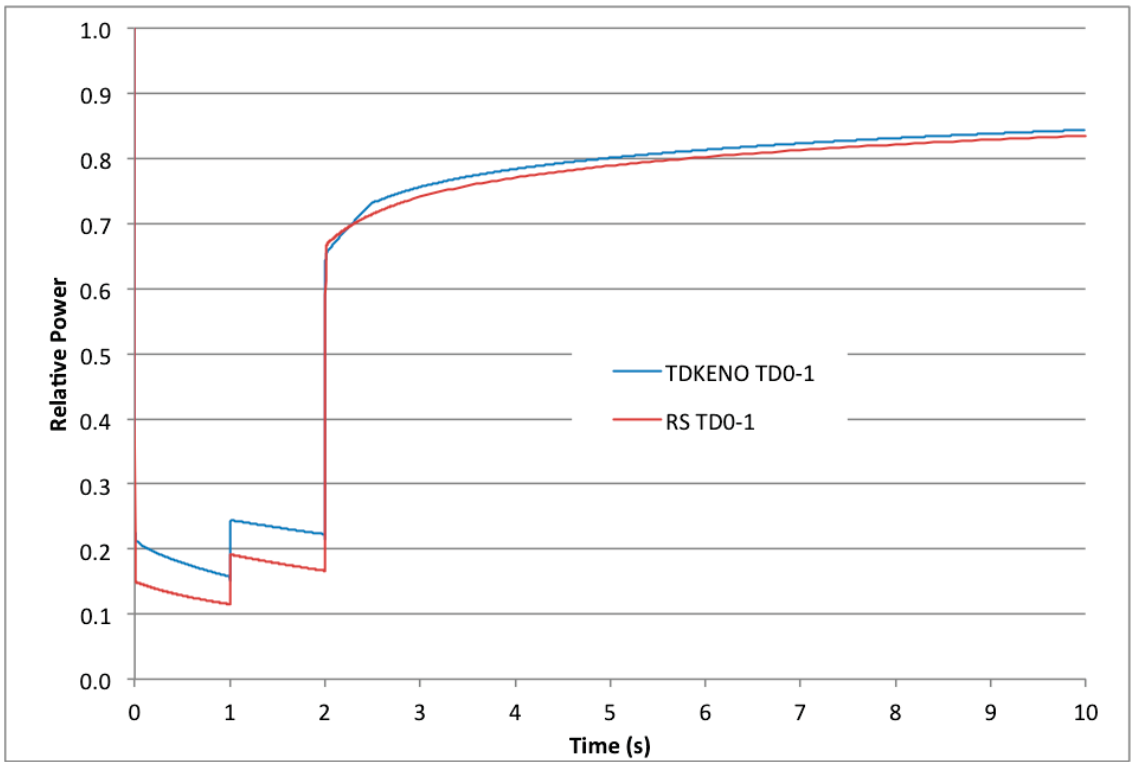

Figure 14: Comparison of Exercise TD0 Case 1 results, Rattlesnake (implicit) vs TD-KENO.

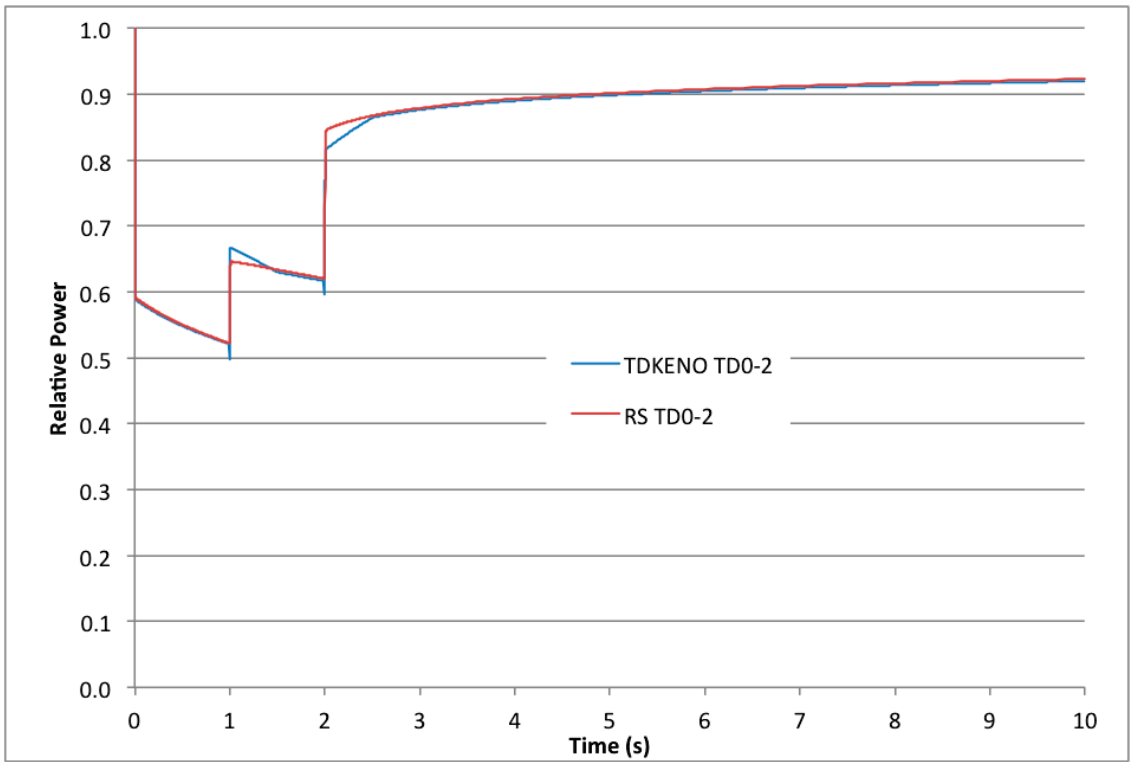

Figure 15: Comparison of Exercise TD0 Case 2 results, Rattlesnake (implicit) vs TD-KENO.

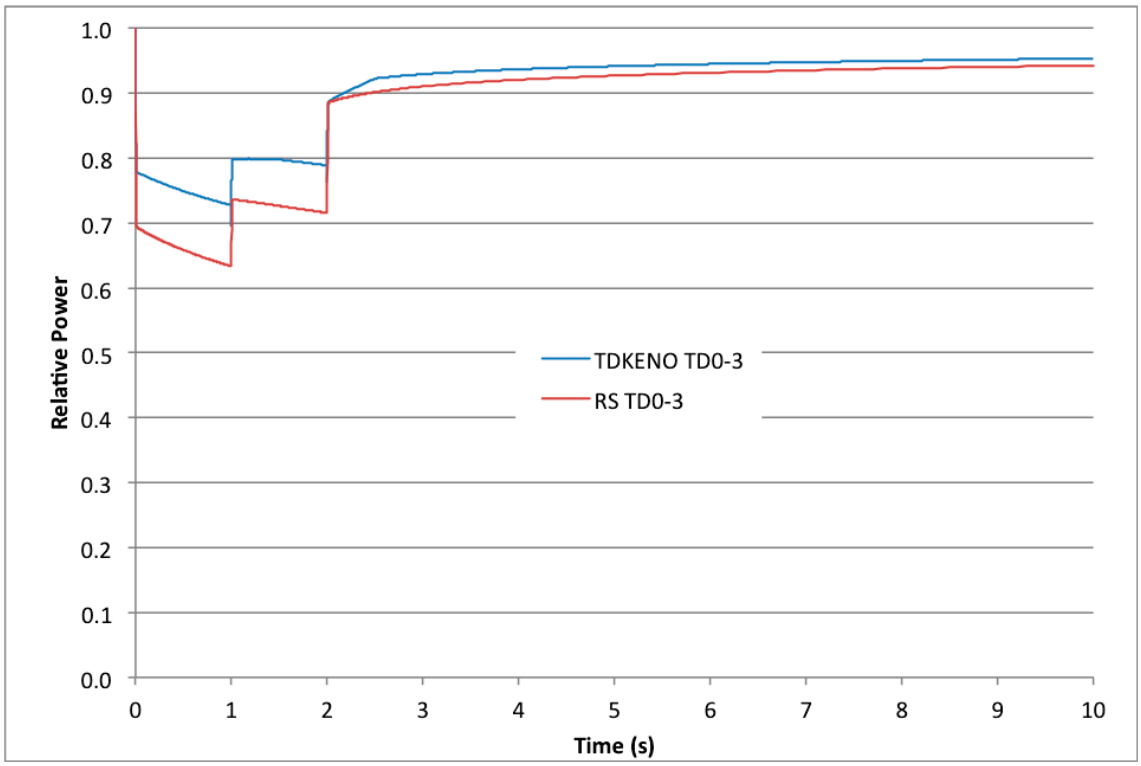

Figure 16: Comparison of Exercise TD0 Case 3 results, Rattlesnake (implicit) vs TD-KENO.

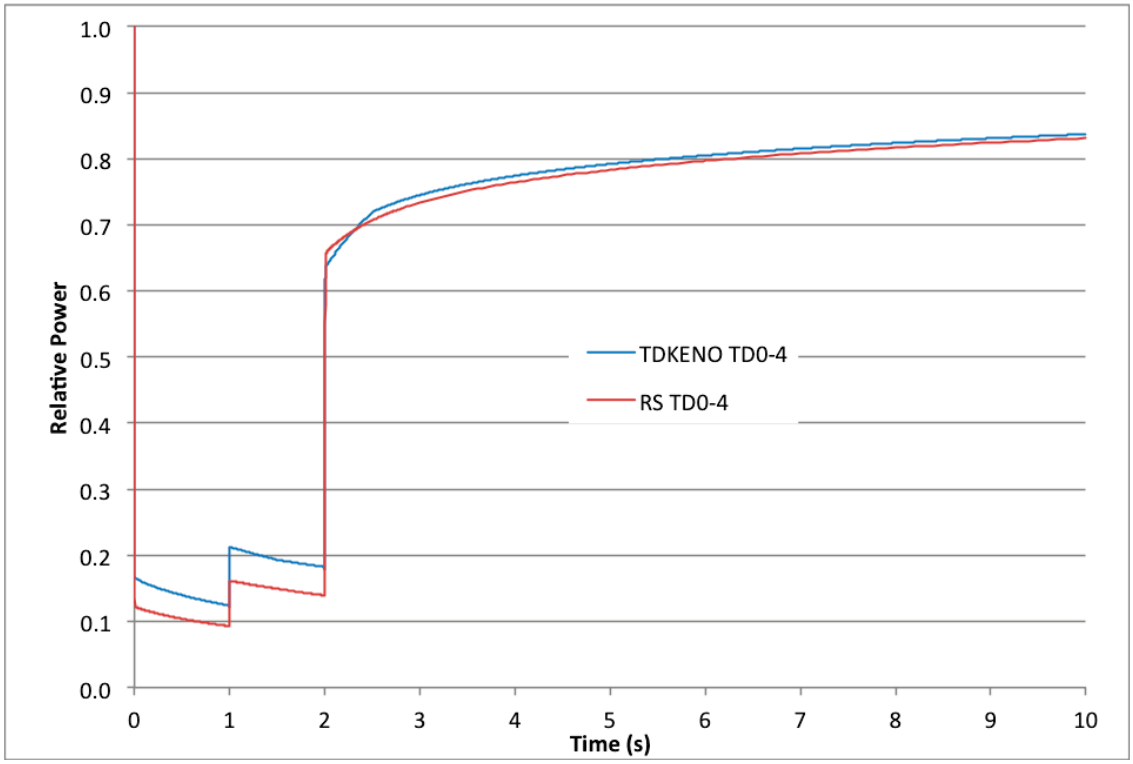

Figure 17: Comparison of Exercise TD0 Case 4 results, Rattlesnake (implicit) vs TD-KENO.

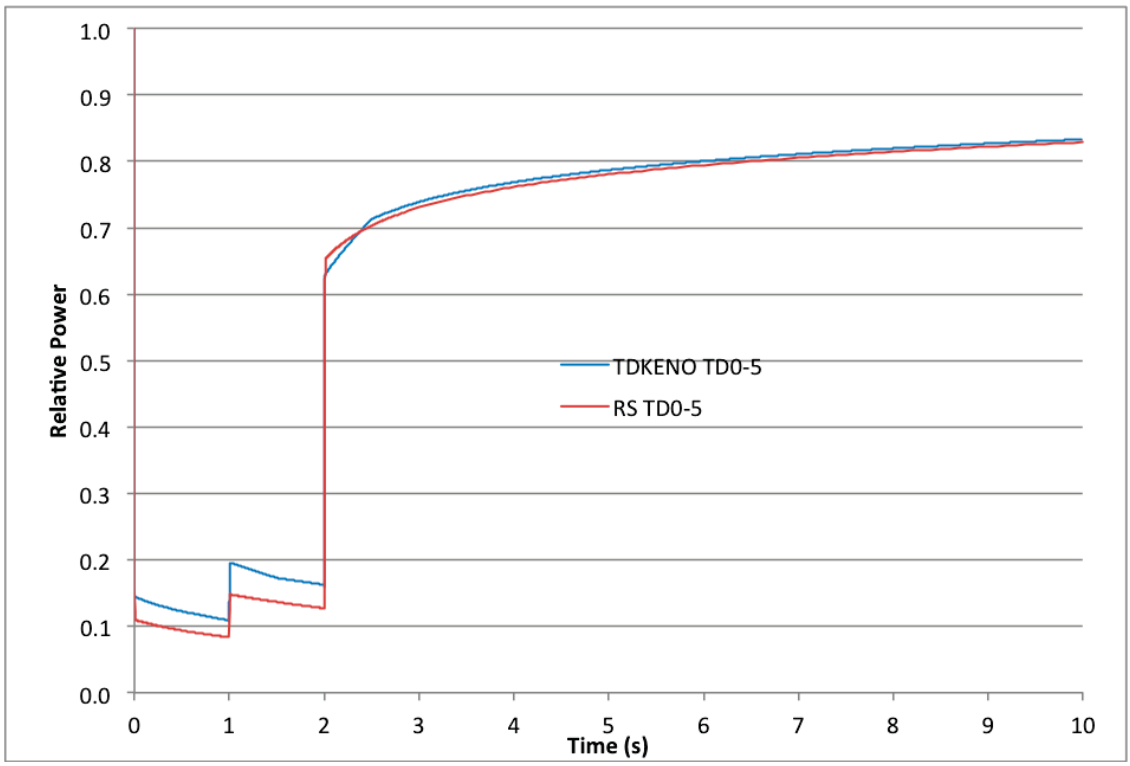

Figure 18: Comparison of Exercise TD0 Case 5 results, Rattlesnake (implicit) vs TD-KENO.

6 Conclusions

The Nuclear Energy Agency of the OECD is sponsoring a time-dependent computational benchmark based on 2D and 3D versions of a well known static benchmark, known as C5G7. The time-dependent specifcation, C5G7-TD, changes the 3D model slightly in the axial specifications. Cross sections and delayed neutron data are provided in the benchmark specification. Calculations will be performed by participating organizations and reported to the benchmark authors. When all submissions have been completed and compiled, an OECD report will be issued to compare the results from all participants. Although not a real or a measured experiment, the comparison of results will show potential weaknesses in some methods, and should show the general concensus for the solution. Thus, this will ultimately provide a general assessment of the performance of the Rattlesnake tranisent solvers.

The benchmark report will not likely be issued for 1-3 years. Thus, it will not provide an international comparison. However, the benchmark does provide a well-specified configuration that can be used to test Rattlesnake performance. In this report, results show that a standard Rattlesnake calculation can successfully simulate the various transient cases, and that the predictions agree with expected performance. Comparisons of the implicit solution to the IQS approximation for a number of benchmark exercises shows very good agreement. It is important to note that although these two methods start at the same initial state, the time-dependent solution algorithms are different and independent.

Work ongoing at the University of Florida using TDKENO seeks to provide a complelely independent approach to confirm the Rattlesnake solution. At this point, comparisons between TDKENO and Rattlesnake have been performed for the Exercise TD0 transients. This is perhaps the most challenging of all the 2D benchmarks, as it uses a step (instantaneous) insertion of negative reactivity. The step insertion results in a corresponding instanteous change in the flux distribution, which is lagged by delayed neutron effects. Lower order kinetics approximations will be challenged by the exercise. And results so far indicate that that instaneous change results in differences between TDKENO and Rattlesnake solutions. Work is ongoing to try to determine why the difference exists, and correct whichever simulation approach is missing the mark.

This effort has been useful in identifying a bug in the IQS solver, which was not initially able to properly represent the the prompt drop in the TD0 cases. This problem was quickly identified and corrected; the results provided here

show that the IQS solution is in remarkable agreement with the implict time-dependent transport simulation in Rattlesnake. Comparisons performed between the two methods for both step and ramped transients show extremely good agreement consistently for the exercises completed. Only a limited number of those comparisons are provided here.

This work will continue into FY17 and all transients will be solved using the three solution methods employed here. This work was based on diffusion solutions; future work will rerun these transients with higher order methods (i.e., S_n and P_n solutions) for the transport solution. Rattlesnake can solve these higher order simulations; the IQS method is currently limited to the diffusion approximation. When higher order IQS solutions become available these problems will be revisited. TDKENO, because it is based on a Monte Carlo solution, represents the highest order solution for the transient. It's weakness results from the need to generate multi-group cross sections for the conditions at the time of the transport solution. UF is studying ways to overcome this limitation, ultimately providing a reference solution against which Rattlesnake (and other codes) can be measure. A followup to this report will be issued near the end of FY17 to describe the state of these analysis, including 3D exercises and higher-order solutions.

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Appendices

Appendix A - C5G7-TD Benchmark Specification,

NEA/NSC/DOC(2016)

Expert Group on Radiation Transport and Shielding (EGRTS) of
Working Party on Scientific Issues of Reactor Systems (WPRS)

Deterministic Time-Dependent Neutron Transport Benchmark without Spatial Homogenization

(C5G7-TD)

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Version 1.6

July 2016

OECD Nuclear Energy Agency

Appendix A

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Appendix A

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.

Appendix A

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 (mini-core): eight uranium oxide (UO_2) 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 17×17 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_2, 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_2 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_2 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

Appendix A

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.

$$\begin{aligned} &\Sigma_x(t) = \Sigma_x^{GT}, t = 0, t \geq 2s \\ &\Sigma_x(t) = \Sigma_x^{GT} + 0.1(\Sigma_x^R - \Sigma_x^{GT}), 0 < t \leq 1s \\ &\Sigma_x(t) = \Sigma_x^{GT} + 0.05(\Sigma_x^R - \Sigma_x^{GT}), 1s \leq t < 2s \end{aligned} \quad (1)$$

where Σ 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.

Appendix A

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:

$$\begin{aligned} &\Sigma_x(t) = \Sigma_x^{GT} + 0.01(\Sigma_x^R - \Sigma_x^{GT})t, 0 \le t < 1s \\ &\Sigma_x(t) = \Sigma_x^{GT} + 0.01(\Sigma_x^R - \Sigma_x^{GT})(2-t), 1s \le t < 2s \\ &\Sigma_x(t) = \Sigma_x^{GT}, t \ge 2s \end{aligned} \quad (2)$$

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):

$$\begin{aligned} &\Sigma_x(t) = \Sigma_x^{GT} + 0.1(\Sigma_x^R - \Sigma_x^{GT})t, 0 \le t < 1s \\ &\Sigma_x(t) = \Sigma_x^{GT} + 0.1(\Sigma_x^R - \Sigma_x^{GT})(2-t), 1s \le t < 2s \\ &\Sigma_x(t) = \Sigma_x^{GT}, t \ge 2s \end{aligned} \quad (3)$$

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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 ω ($0 \leq \omega \leq 1$), 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 ω 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.

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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.

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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.

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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 cross sections uniformly in all fuel regions; that is, dividing the fission cross section or Nu by the core k_{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 used in 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.

Note that the fission rate distribution should be normalized in such a way that the average value across the core is equal to the fractional total core fission rate at a given time point.

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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.

Appendix A

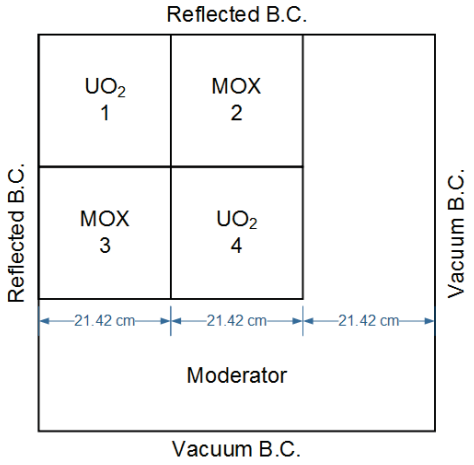


Figure 1. 2-D configuration for the C5G7 benchmark problem

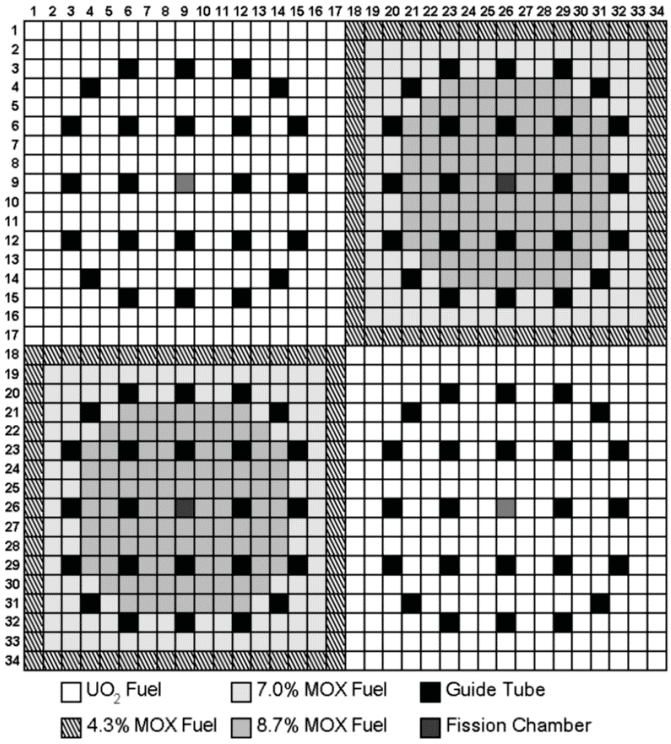


Figure 2. C5G7 fuel pin compositions and numbering scheme

Appendix A

Figure 3. C5G7 pin cell layout

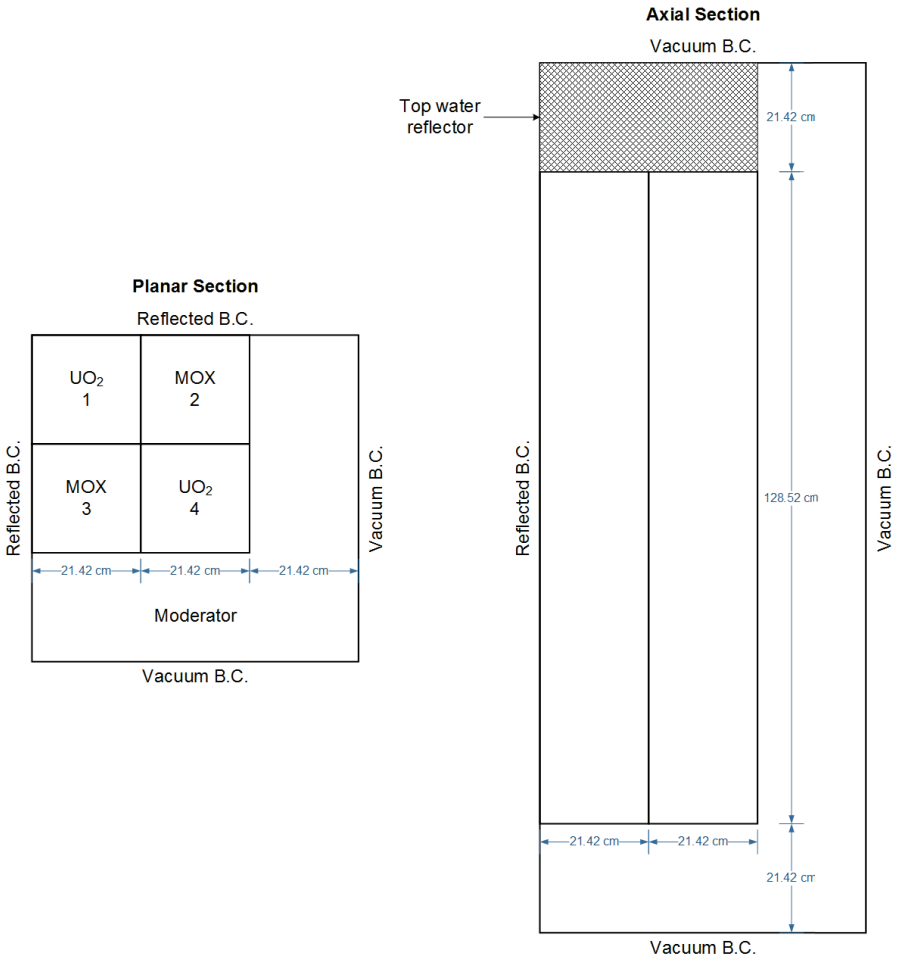


Figure 4. Modified 3-D configuration for the benchmark problem

Appendix A

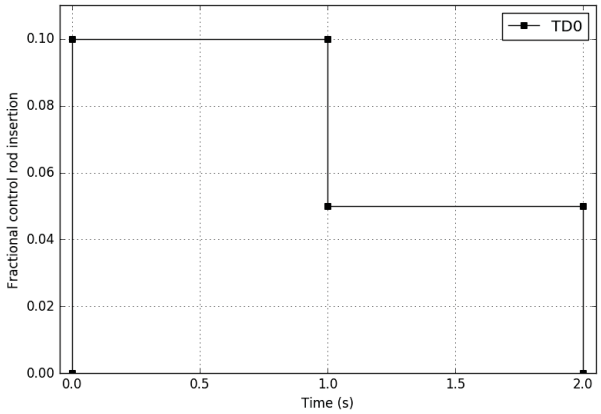


Figure 5. Control rod movement in TD0 transient exercise

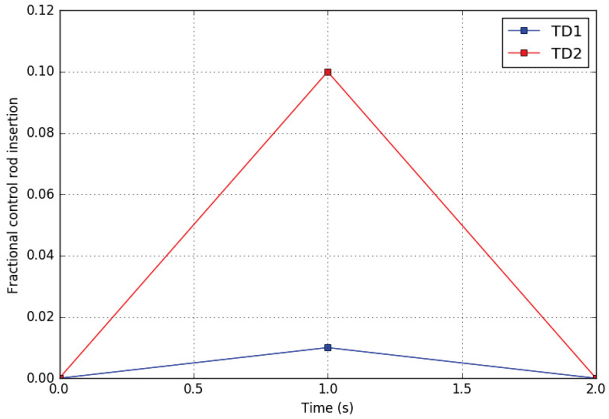


Figure 6. Control rod movement in transient exercise TD1 and TD2

Appendix A

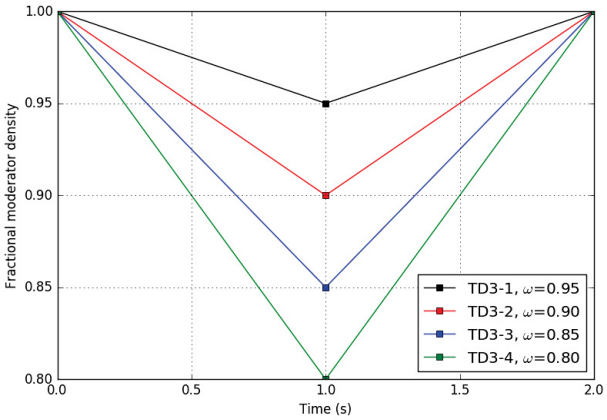


Figure 7. Core average moderator density change in TD3 exercises

Appendix A

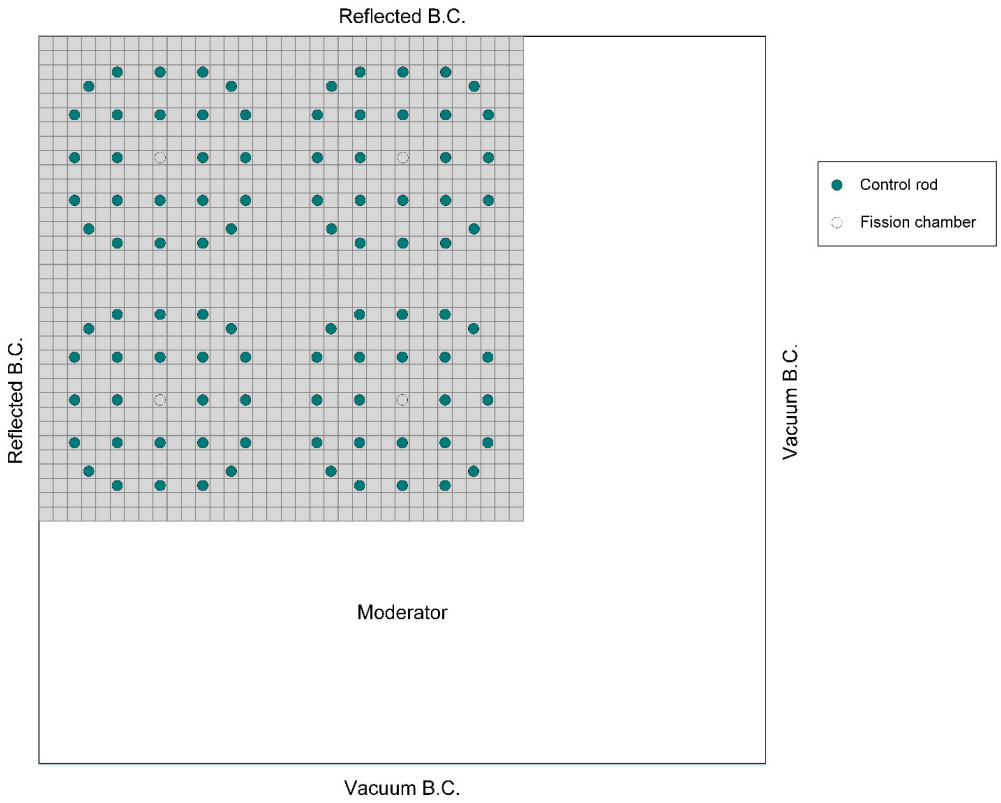
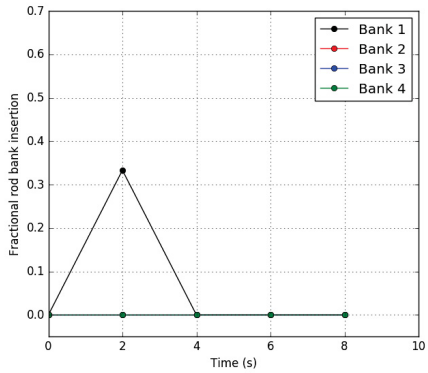
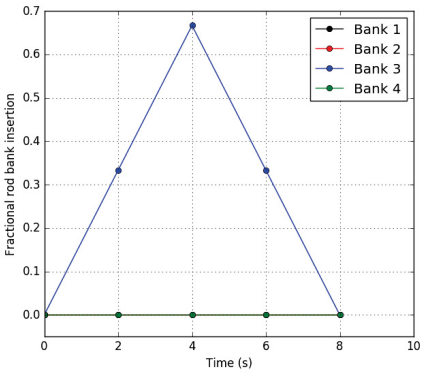


Figure 8. Geometry configuration for the top water reflector

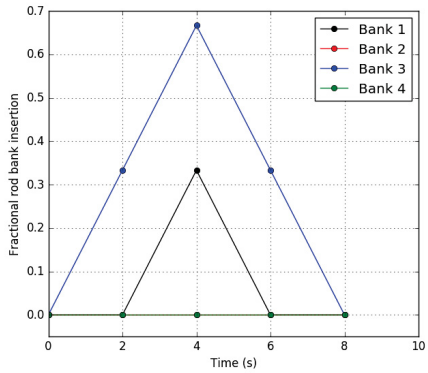
Appendix A



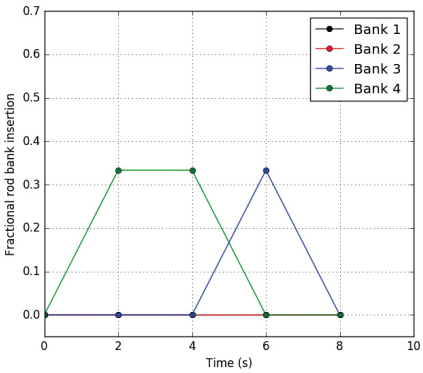
TD4-1



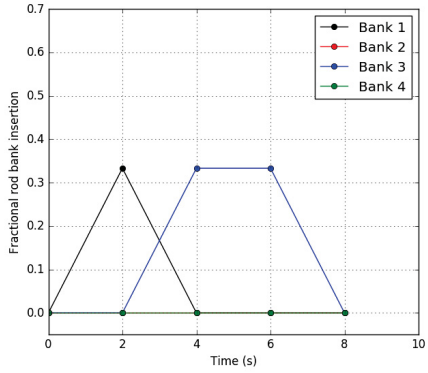
TD4-2



TD4-3



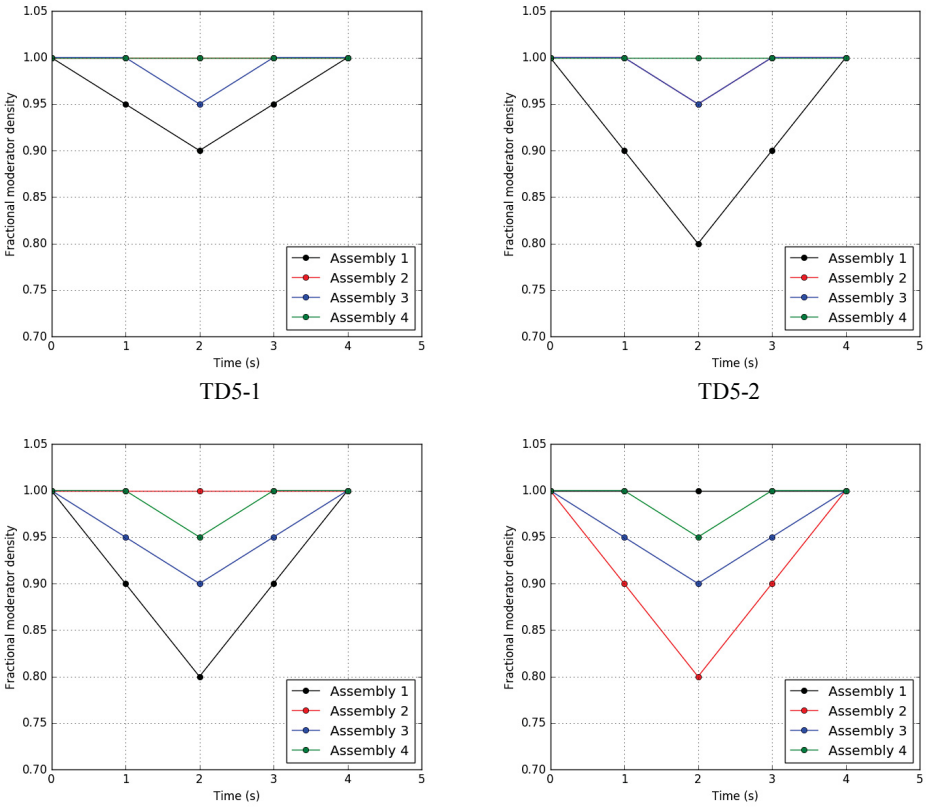
TD4-4



TD4-5

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

Appendix A



TD5-1 TD5-2

TD5-3 TD5-4

Figure 10. Relative moderator density in TD5 exercise

Appendix A

References

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Appendix A

Appendix I Macroscopic cross sections and kinetics parameters

Table 1. UO_2 fuel-clad macroscopic cross sections

Group	Transport cross section (cm^{-1})	Absorption cross section (cm^{-1})	Capture cross section (cm^{-1})	Fission cross section (cm^{-1})	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^{-1})

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

Group	Transport cross section (cm^{-1})	Absorption cross section (cm^{-1})	Capture cross section (cm^{-1})	Fission cross section (cm^{-1})	Nu	Chi
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^{-1})

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

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

Group	Transport cross section (cm^{-1})	Absorption cross section (cm^{-1})	Capture cross section (cm^{-1})	Fission cross section (cm^{-1})	Nu	Chi
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	2.44666E-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^{-1})

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

Group	Transport cross section (cm^{-1})	Absorption cross section (cm^{-1})	Capture cross section (cm^{-1})	Fission cross section (cm^{-1})	Nu	Chi
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	3.74888E-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^{-1})

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

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Table 5. Fission chamber macroscopic cross sections

Group	Transport cross section (cm^{-1})	Absorption cross section (cm^{-1})	Capture cross section (cm^{-1})	Fission cross section (cm^{-1})	Nu	Chi
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^{-1})

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^{-1})

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

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

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Table 7. Moderator macroscopic cross sections (unit: cm^{-1})

Group	Transport cross section	Absorption cross section	Capture 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^{-1})

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^{-1})

Group	Transport cross section	Absorption cross section	Capture 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^{-1})

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

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Table 9. Delayed neutron fractions

Delayed neutron group	UO_2	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

Delayed neutron group	UO_2	MOX 4.3%	MOX 7.0%	MOX 8.7%
1	1.247E-02	1.247E-02	1.247E-02	1.247E-02
2	2.829E-02	2.829E-02	2.829E-02	2.829E-02
3	4.252E-02	4.252E-02	4.252E-02	4.252E-02
4	1.330E-01	1.330E-01	1.330E-01	1.330E-01
5	2.925E-01	2.925E-01	2.925E-01	2.925E-01
6	6.665E-01	6.665E-01	6.665E-01	6.665E-01
7	1.635E+00	1.635E+00	1.635E+00	1.635E+00
8	3.555E+00	3.555E+00	3.555E+00	3.555E+00

Table 11. Delayed neutron group spectra

g \ *i*	1	2	3	4	5	6	7	8
	UO_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

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g \ *i*	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

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Appendix II Original cell geometry and composition

Table 14. Pin cell geometries

Fuel cells: MOX 4.3%, MOX 7.0%, MOX8.7% and UO_2

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

* 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 ^{235}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)

Nuclide	Concentrations (10^{24} at/cm^3)						
	MOX 4.3%	MOX 7.0%	MOX 8.7%	UO_2	Moderator	Zr Clad	Al Clad
^{235}U	5.0000E-5	5.0000E-5	5.0000E-5	8.6500E-4			
^{238}U	2.2100E-2	2.2100E-2	2.2100E-2	2.2250E-2			
^{238}Pu	1.5000E-5	2.4000E-5	3.0000E-5				
^{239}Pu	5.8000E-4	9.3000E-4	1.1600E-3				
^{240}Pu	2.4000E-4	3.9000E-4	4.9000E-4				
^{241}Pu	9.8000E-5	1.5200E-4	1.9000E-4				
^{242}Pu	5.4000E-5	8.4000E-5	1.0500E-4				
^{241}Am	1.3000E-5	2.0000E-5	2.5000E-5				
O	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	
^{27}Al							6.0000E-2

Table 16. Isotopic distribution for control rod cell

Nuclide	Concentrations (10^{24} at/cm^3)		
	Absorber	Moderator	Al cladding
^{107}Ag	2.27105E-2		
^{109}Ag	2.27105E-2		
^{115}In	8.00080E-3		
^{113}Cd	2.72410E-3		
H_2O		3.3500E-2	
B nat		2.7800E-5	
^{27}Al			6.0000E-2

Appendix A

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_{eff} (or k_d) will be automatically calculated based on the input core reactivity, as shown in the 3rd 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 time [s]	Core reactivity ρ [pcm]	Core dynamic multiplication factor k_d	Fractional total core fission rate P	Effective delayed neutron fraction β_{eff}	Prompt neutron 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

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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	1.000	1.000
2	1.000	1.000

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	1.000	1.000	1.000	1.000	1.000	1.000
2	1.000	1.000	1.000	1.000	1.000	1.000
3	1.000	1.000	1.000	1.000	1.000	1.000
…	…	…	…	…	…	…
33	1.000	1.000	1.000	1.000	1.000	1.000
34	1.000	1.000	1.000	1.000	1.000	1.000

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	1.000	1.000
	2	1.000	1.000
…	1	1.000	1.000
	2	1.000	1.000
10.710	…	…	…
5.355	1	1.000	1.000
	2	1.000	1.000

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
128.520	1	1.000	1.000	1.000	1.000	1.000	1.000
	2	1.000	1.000	1.000	1.000	1.000	1.000
	3	1.000	1.000	1.000	1.000	1.000	1.000
	…	…	…	…	…	…	…
	33	1.000	1.000	1.000	1.000	1.000	1.000
	34	1.000	1.000	1.000	1.000	1.000	1.000
…	…	…	…	…	…	…	…
10.710	1	1.000	1.000	1.000	1.000	1.000	1.000
	2	1.000	1.000	1.000	1.000	1.000	1.000

Appendix A

	3	1.000	1.000	1.000	1.000	1.000	1.000
	…	…	…	…	…	…	…
	33	1.000	1.000	1.000	1.000	1.000	1.000
	34	1.000	1.000	1.000	1.000	1.000	1.000
Axial position [cm]	Row\ Column	1	2	3	…	33	34
5.355	1	1.000	1.000	1.000	1.000	1.000	1.000
	2	1.000	1.000	1.000	1.000	1.000	1.000
	3	1.000	1.000	1.000	1.000	1.000	1.000
	…	…	…	…	…	…	…
	33	1.000	1.000	1.000	1.000	1.000	1.000
	34	1.000	1.000	1.000	1.000	1.000	1.000

Appendix A

Appendix IV Additional definitions

Cumulative fission spectrum

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

$$\begin{aligned}\frac{1}{v}\frac{\partial\psi(\mathrm{w})}{\partial t}+\Omega\cdot\nabla\psi(\mathrm{w})+\Sigma(r,E,t)\psi(w)&\\ =\int\int\Sigma_s(r,t,\Omega',E'\to\Omega,E)\psi(w')d\Omega'\,dE'&\\ +\tilde{\chi}_p(E)\int\int[1-\beta(r,E')]v\Sigma_f(r,E',t)\psi(w')d\Omega'\,dE'&\\ +\sum_j\tilde{\chi}_j(E)\lambda_jC_j(r,t)&\end{aligned}\tag{4}$$

and

$$\frac{\partial C_j(\mathrm{r,t})}{\partial t}=-\lambda_jC_j(r,t)+\int\int\beta_j(r,E')v\Sigma_f(r,E',t)\psi(w')d\Omega'\,dE'\tag{5}$$

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,

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

$\beta(\mathrm{r}, E')$ = total delayed neutron fraction and $\beta(r,E')=\sum_j\beta_j(r,E')$,

$C_j(\mathrm{r}, t)$ = 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

$$\begin{aligned}\tilde{\chi}_{cum}(E)\int\int v\Sigma_f(r,E',t)\psi(w')d\Omega'\,dE'&\\ =\tilde{\chi}_p(E)\int\int[1-\beta(r,E')]v\Sigma_f(r,E',t)\psi(w')d\Omega'\,dE'&\\ +\sum_j\tilde{\chi}_j(E)\int\int\beta_j(r,E')v\Sigma_f(r,E',t)\psi(w')d\Omega'\,dE'&\end{aligned}\tag{6}$$

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:

[*] Bell, George I., and Samuel Glasstone. Nuclear Reactor Theory. No. TID--25606. Division of Technical Information, US Atomic Energy Commission, 1970.

Appendix A

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

and the reactivity can be written as

$$\rho(t) = \frac{1}{F(t)}\left\{\int \dots \int \Delta\left[\sum_{x\neq f}\Sigma_x f_x(r;\Omega',E'\to\Omega,E;t) + \tilde{\chi}_{cum}(E)\nu\Sigma_f(r,E,t)\right] \times \psi(r,\Omega',E',t)\Phi_0^+(r,\Omega,E)dVd\Omega dEd\Omega' dE' - \iiint \Delta\Sigma(r,E,t)\psi(r,\Omega,E,t)\Phi_0^+(r,\Omega,E)\right\} \tag{8}$$

where Φ_0^+ is the adjoint function, which is defined as the fundamental mode eigenfunction of the equation adjoint to the time independent transport equation. The Δ's represent the differences between the respective quantities, *Σf* and *Σ*, in the time-varying state and in the time-independent (critical) reference state, e.g., $\Delta\Sigma = \Sigma - \Sigma_0$.

Effective delayed neutron fraction

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

$$\bar{\beta}_j(t) = \frac{1}{F(t)}\int \dots \int \tilde{\chi}_j(E)\beta_j\nu\Sigma_f(r,E',t)\psi(r,\Omega',E',t)\Phi_0^+(r,\Omega,E)dVd\Omega dEd\Omega'\,dE' \tag{9}$$

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

$$\bar{\beta}(t) = \sum\nolimits_j \bar{\beta}_j(t) \tag{10}$$

Prompt neutron lifetime

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

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

Appendix B - INSTANT Input for C5G7-TD Mesh,

```
<task type="generation">
  <!--
    Description of the mesh
  -->
  <Geometry type="LWR">
    <Controls>
      <MaxArea>0.064</MaxArea>
      <PinMaxArea>0.256</PinMaxArea>
      <AssemblyMaxArea>4.096</AssemblyMaxArea>
      <MinAngle>20</MinAngle>
      <DebugOutput>t</DebugOutput>
      <BlockOption>0</BlockOption>
    </Controls>
    <Pins>
      <Pin ID="1" shape="cylindrical" type="full" name="UO2">
        <Radius>0.54 0.63</Radius>
        <MaterialID>1 7</MaterialID>
        <NSides>8</NSides><Rotation>0</Rotation>
      </Pin>
      <Pin ID="2" shape="cylindrical" type="full" name="MOX4.3">
        <Radius>0.54 0.63</Radius>
        <MaterialID>2 7</MaterialID>
        <NSides>8</NSides><Rotation>0</Rotation>
      </Pin>
      <Pin ID="3" shape="cylindrical" type="full" name="MOX7.0">
        <Radius>0.54 0.63</Radius>
        <MaterialID>3 7</MaterialID>
        <NSides>8</NSides><Rotation>0</Rotation>
    </Pin>
  <Pin ID="4" shape="cylindrical" type="full" name="MOX8.7">
    <Radius>0.54 0.63</Radius>
    <MaterialID>4 7</MaterialID>
    <NSides>8</NSides><Rotation>0</Rotation>
  </Pin>
  <Pin ID="15" shape="cylindrical" type="full" name="Guide Tube
Z1">
    <Radius>0.54 0.63</Radius>
    <MaterialID>15 7</MaterialID>
    <NSides>8</NSides><Rotation>0</Rotation>
  </Pin>
  <Pin ID="25" shape="cylindrical" type="full" name="Guide Tube
Z2">
    <Radius>0.54 0.63</Radius>
    <MaterialID>25 7</MaterialID>
    <NSides>8</NSides><Rotation>0</Rotation>
  </Pin>
```

Appendix B

```
  <Pin ID="35" shape="cylindrical" type="full" name="Guide Tube
Z3">
    <Radius>0.54 0.63</Radius>
    <MaterialID>35 7</MaterialID>
    <NSides>8</NSides><Rotation>0</Rotation>
  </Pin>
  <Pin ID="45" shape="cylindrical" type="full" name="Guide Tube
Z4">
    <Radius>0.54 0.63</Radius>
    <MaterialID>45 7</MaterialID>
    <NSides>8</NSides><Rotation>0</Rotation>
  </Pin>
  <Pin ID="6" shape="cylindrical" type="full" name="Fission
Chamber">
    <Radius>0.54 0.63</Radius>
    <MaterialID>6 7</MaterialID>
    <NSides>8</NSides><Rotation>0</Rotation>
  </Pin>
  <Pin ID="7" shape="rectangular" name="Reflector">
    <NX>1</NX><NY>1</NY><IX>1</IX><IY>1</IY>
    <DX>1.26</DX><DY>1.26</DY>
    <MaterialID>7</MaterialID>
  </Pin>
</Pins>
<Assemblies>
  <Assembly ID="1" name="UO2 Z1">
    <NXPin>17</NXPin><NYPin>17</NYPin>
    <PinArrangement>
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1 15  1  1 15  1  1 15  1  1  1  1  1
1  1  1 15  1  1  1  1  1  1  1  1  1 15  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1 15  1  1 15  1  1 15  1  1 15  1  1 15  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1 15  1  1 15  1  1  6  1  1 15  1  1 15  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1 15  1  1 15  1  1 15  1  1 15  1  1 15  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1 15  1  1  1  1  1  1  1  1  1 15  1  1  1
1  1  1  1  1 15  1  1 15  1  1 15  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
    </PinArrangement>
```

Appendix B

```
    <XT>21.42</XT><YT>21.42</YT>
  </Assembly>
  <Assembly ID="2" name="MOX Z2">
    <NXPin>17</NXPin><NYPin>17</NYPin>
    <PinArrangement>
2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
2  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  2
2  3  3  3  3 25  3  3 25  3  3 25  3  3  3  3  2
2  3  3 25  3  4  4  4  4  4  4  4  3 25  3  3  2
2  3  3  3  4  4  4  4  4  4  4  4  4  3  3  3  2
2  3 25  4  4 25  4  4 25  4  4 25  4  4 25  3  2
2  3  3  4  4  4  4  4  4  4  4  4  4  4  3  3  2
2  3  3  4  4  4  4  4  4  4  4  4  4  4  3  3  2
2  3 25  4  4 25  4  4  6  4  4 25  4  4 25  3  2
2  3  3  4  4  4  4  4  4  4  4  4  4  4  3  3  2
2  3  3  4  4  4  4  4  4  4  4  4  4  4  3  3  2
2  3 25  4  4 25  4  4 25  4  4 25  4  4 25  3  2
2  3  3  3  4  4  4  4  4  4  4  4  4  3  3  3  2
2  3  3 25  3  4  4  4  4  4  4  4  3 25  3  3  2
2  3  3  3  3 25  3  3 25  3  3 25  3  3  3  3  2
2  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  2
2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
      </PinArrangement>
      <XT>21.42</XT><YT>21.42</YT>
    </Assembly>
  <Assembly ID="3" name="MOX Z3">
    <NXPin>17</NXPin><NYPin>17</NYPin>
    <PinArrangement>
2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
2  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  2
2  3  3  3  3 35  3  3 35  3  3 35  3  3  3  3  2
2  3  3 35  3  4  4  4  4  4  4  4  3 35  3  3  2
2  3  3  3  4  4  4  4  4  4  4  4  4  3  3  3  2
2  3 35  4  4 35  4  4 35  4  4 35  4  4 35  3  2
2  3  3  4  4  4  4  4  4  4  4  4  4  4  3  3  2
2  3  3  4  4  4  4  4  4  4  4  4  4  4  3  3  2
2  3 35  4  4 35  4  4  6  4  4 35  4  4 35  3  2
2  3  3  4  4  4  4  4  4  4  4  4  4  4  3  3  2
2  3  3  4  4  4  4  4  4  4  4  4  4  4  3  3  2
2  3 35  4  4 35  4  4 35  4  4 35  4  4 35  3  2
2  3  3  3  4  4  4  4  4  4  4  4  4  3  3  3  2
2  3  3 35  3  4  4  4  4  4  4  4  3 35  3  3  2
2  3  3  3  3 35  3  3 35  3  3 35  3  3  3  3  2
2  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  2
2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2  2
      </PinArrangement>
```

```
        <XT>21.42</XT><YT>21.42</YT>
      </Assembly>
  <Assembly ID="4" name="UO2 Z4">
    <NXPin>17</NXPin><NYPin>17</NYPin>
    <PinArrangement>
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1 45  1  1 45  1  1 45  1  1  1  1  1
1  1  1 45  1  1  1  1  1  1  1  1  1 45  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1 45  1  1 45  1  1 45  1  1 45  1  1 45  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1 45  1  1 45  1  1  6  1  1 45  1  1 45  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1 45  1  1 45  1  1 45  1  1 45  1  1 45  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1 45  1  1  1  1  1  1  1  1  1 45  1  1  1
1  1  1  1  1 45  1  1 45  1  1 45  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
    </PinArrangement>
    <XT>21.42</XT><YT>21.42</YT>
  </Assembly>
      <Assembly ID="5" name="Reflector">
        <NXPin>17</NXPin><NYPin>17</NYPin>
        <PinArrangement>
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
 7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7  7
        </PinArrangement>
```

Appendix B

```
        <XT>21.42</XT><YT>21.42</YT>
      </Assembly>
    </Assemblies>
    <Core name="C5G7">
      <BC>1 0 1 0</BC>
      <NX>3</NX><NY>3</NY>
      <Layout>
1 2 5
3 4 5
5 5 5
</Layout>
<Homogenization>
0 0 0
0 0 0
0 0 0
</Homogenization>
    </Core>
  </Geometry>
  <!--
    1-15 for generating blocks
  -->
  <option>3</option>
  <output>c5g7-td-2d-base.e</output>
</task>
```

Appendix C - Rattlesnake input for 3D extrusion of 2D C5G7-TD Mesh,

```
[Mesh]
 file = c5g7-td-2d-base.e
[]

[MeshModifiers]
  [./extrude]
    type = MeshExtruder
    num_layers = 32
    extrusion_vector = '0 0 171.36'
    bottom_sideset = 'core_bot'
    top_sideset = 'core_top'
#    existing_subdomains = '7 1 15 6 2 3 35 4 25 45'
    existing_subdomains = ' 1 2 3  4 5 6 7  8 9  10'

    layers = '0 1 2 3 28 29 30 31'
    new_ids = '1 1 18 4 1 1 38 1 28 48
               1 1 18 4 1 1 38 1 28 48
               1 1 18 4 1 1 38 1 28 48
               1 1 18 4 1 1 38 1 28 48
               1 1 1 1 1 1 1 1 1 1
               1 1 1 1 1 1 1 1 1 1
               1 1 1 1 1 1 1 1 1 1
               1 1 1 1 1 1 1 1 1 1'
  [../]
  [./RenameBlock]
    depends_on = extrude
    type = RenameBlock
    old_block_id = '18 28 38 48'
    new_block_name = 'M-18-TRI M-28-TRI M-38-TRI M-48-TRI'
  [../]
[]
```

Appendix D - Rattlesnake Input for All 2D Eigenvalue Calculations,

```
[Mesh]
 file = c5g7-td-2d-base.e
[]

[TransportSystems]
  particle = neutron
  G = 7
  VacuumBoundary = 'vacuum'
  ReflectingBoundary = 'reflecting'
  equation_type = eigenvalue
  [./diffusion]
    order = FIRST
    n_delay_groups = 8
    scheme = CFEM-Diffusion
  [../]
[]

[GlobalParams]
  fromFile = true
  fileName = ./c5g7_materials_critical.xml
  plus = true
[]

 [AuxVariables]
   [./power]
     order=FIRST
     family = MONOMIAL
   [../]
 []

 [AuxKernels]
   [./power]
     type = VectorReactionRate
     scalar_flux = 'sflux_g0 sflux_g1 sflux_g2 sflux_g3 sflux_g4
sflux_g5 sflux_g6'
     cross_section = kappa_sigma_fission
     variable = power
     block ='M-1-TRI M-2-TRI M-3-TRI M-4-TRI'
     execute_on = linear
   [../]
 []

[Materials]
  [./uo2]
    type = ConstantNeutronicsMaterial
    block = 'M-1-TRI'
```

Appendix D

```
  material_id = 1
[../]
[./mox4.3]
  type = ConstantNeutronicsMaterial
  block = 'M-2-TRI'
  material_id = 2
[../]
[./mox7.0]
  type = ConstantNeutronicsMaterial
  block = 'M-3-TRI'
  material_id = 3
[../]
[./mox8.7]
  type = ConstantNeutronicsMaterial
  block = 'M-4-TRI'
  material_id = 4
[../]
[./GuideTube_Z1]
  type = ConstantNeutronicsMaterial
  block = 'M-15-TRI'
  material_id = 5
[../]
[./GuideTube_Z2]
  type = ConstantNeutronicsMaterial
  block = 'M-25-TRI'
  material_id = 5
[../]
[./GuideTube_Z3]
  type = ConstantNeutronicsMaterial
  block = 'M-35-TRI'
  material_id = 5
[../]
[./GuideTube_Z4]
  type = ConstantNeutronicsMaterial
  block = 'M-45-TRI'
  material_id = 5
[../]
[./FissionChamber_Z1]
  type = ConstantNeutronicsMaterial
  block = 'M-6-TRI'
  material_id = 6
[../]
[./moderator]
  type = ConstantNeutronicsMaterial
  block = 'M-7-TRI'
  material_id = 7
```

Appendix D

```
  [../]
[]

[Postprocessors]
  [./runtime]
    type = RunTime
    time_type = alive
  [../]
[]

[Executioner]
  type = NonlinearEigen
  solve_type = 'PJFNK'
  petsc_options_iname = '-pc_type -pc_hypre_type -
ksp_gmres_restart '
  petsc_options_value = 'hypre boomeramg 100'
  free_power_iterations = 5
  source_abs_tol = 1e-10
[]

[Postprocessors]
   [./avg_power]
     type = ElementAverageValue
     execute_on = 'initial timestep_end'
     variable = power
     block = 'M-1-TRI M-2-TRI M-3-TRI M-4-TRI'
     outputs = none
   [../]
   [./power]
     type = ScalePostprocessor
     execute_on = 'initial timestep_end'
     value = avg_power
     scaling_factor = 2141.4381
   [../]
  [./runtime]
    type = RunTime
    time_type = alive
  [../]
[]


[Outputs]
  file_base = c5g7-td_initial
  exodus = true
  csv = true
[]
```

Appendix E - Sample Rattlesnake Input (TD0.1),

```
[Mesh]
 file = c5g7-td-2d-base.e
[]

[TransportSystems]
  particle = neutron
  G = 7
  VacuumBoundary = 'vacuum'
  ReflectingBoundary = 'reflecting'
  equation_type = transient
  [./diffusion]
    order = FIRST
    n_delay_groups = 8
    scheme = CFEM-Diffusion
  [../]
[]

[GlobalParams]
  fromFile = true
  fileName = ./c5g7_materials_critical.xml
  plus = true
[]

[Materials]
  [./uo2]
    type = ConstantNeutronicsMaterial
    block = 'M-1-TRI'
    material_id = 1
  [../]
  [./mox4.3]
    type = ConstantNeutronicsMaterial
    block = 'M-2-TRI'
    material_id = 2
  [../]
  [./mox7.0]
    type = ConstantNeutronicsMaterial
    block = 'M-3-TRI'
    material_id = 3
  [../]
  [./mox8.7]
    type = ConstantNeutronicsMaterial
    block = 'M-4-TRI'
    material_id = 4
  [../]
  [./GuideTube_Z1]
    type = CRoddedNeutronicsMaterial
```

Appendix E

```
    block = 'M-15-TRI'
    position_as_fraction = true
    material_ids = '8 5'
    front_position_function = rodMove
  [../]
  [./GuideTube_Z2]
    type = ConstantNeutronicsMaterial
    block = 'M-25-TRI'
    material_id = 5
  [../]
  [./GuideTube_Z3]
    type = ConstantNeutronicsMaterial
    block = 'M-35-TRI'
    material_id = 5
  [../]
  [./GuideTube_Z4]
    type = ConstantNeutronicsMaterial
    block = 'M-45-TRI'
    material_id = 5
  [../]
  [./FissionChamber]
    type = ConstantNeutronicsMaterial
    block = 'M-6-TRI'
    material_id = 6
  [../]
  [./moderator]
    type = ConstantNeutronicsMaterial
    block = 'M-7-TRI'
    material_id = 7
  [../]
[]

[MultiApps]
 [./initial_solve]
   type = FullSolveMultiApp
   execute_on = initial
   input_files = c5g7-td_initial.i
 [../]
[]

[Transfers]
 [./copy_solution]
   type = TransportSystemVariableTransfer
   from_transport_system = diffusion
   to_transport_system = diffusion
   direction = from_multiapp
```

Appendix E

```
    multi_app = initial_solve
    execute_on = initial
  [../]
 []

 [AuxVariables]
   [./power]
     order=FIRST
     family = MONOMIAL
   [../]
  [./adjoint_flux_g0]
    family = LAGRANGE
    order = FIRST
    initial_condition = 1
  [../]
  [./adjoint_flux_g1]
    family = LAGRANGE
    order = FIRST
    initial_condition = 1
  [../]
  [./adjoint_flux_g2]
    family = LAGRANGE
    order = FIRST
    initial_condition = 1
  [../]
  [./adjoint_flux_g3]
    family = LAGRANGE
    order = FIRST
    initial_condition = 1
  [../]
  [./adjoint_flux_g4]
    family = LAGRANGE
    order = FIRST
    initial_condition = 1
  [../]
  [./adjoint_flux_g5]
    family = LAGRANGE
    order = FIRST
    initial_condition = 1
  [../]
  [./adjoint_flux_g6]
    family = LAGRANGE
    order = FIRST
    initial_condition = 1
  [../]
 []
```

Appendix E

```
 [AuxKernels]
   [./power]
     type = VectorReactionRate
     scalar_flux = 'sflux_g0 sflux_g1 sflux_g2 sflux_g3 sflux_g4
sflux_g5 sflux_g6'
     cross_section = kappa_sigma_fission
     variable = power
     block ='M-1-TRI M-2-TRI M-3-TRI M-4-TRI'
     execute_on = linear
   [../]
 []

[Functions]
  [./rodMove]
#  TD0
    type = StepFunction
    timep = '0.0 1.0 2.0'
    value = '0.0 0.01 0.005 0.0'
  [../]
[]
[Postprocessors]
   [./avg_power]
     type = ElementAverageValue
     execute_on = 'initial timestep_end'
     variable = power
     block = 'M-1-TRI M-2-TRI M-3-TRI M-4-TRI'
   [../]
   [./power]
     type = ScalePostprocessor
     execute_on = 'initial timestep_end'
     value = avg_power
     scaling_factor = 2141.4381
   [../]
  [./runtime]
    type = RunTime
    time_type = alive
  [../]
[]

[Executioner]
   type = IQS
   do_iqs_transient = false
   pke_param_csv = c5g7-td0.1_params.csv

   start_time = 0
```

Appendix E

```
   end_time = 10.0
   [./TimeStepper]
     cutback_factor           = 0.5
     dt                       = 0.001
     enable                   = true
     force_step_every_function_point = true
     growth_factor            = 2
     time_dt                  = '0.001 0.002 0.01  0.01 0.001
0.002 0.01 0.01 0.001 0.002 0.01 0.01  0.05 0.05 0.05 0.1 0.1
0.1 0.1 0.1'
     time_t                   = '0.0   0.25  0.50  0.75 1.0
1.25  1.5  1.75 2.0   2.25  2.5  2.75  3.0  4.0  5.0  6.0 7.0
8.0 9.0 10.0'
     type                     = IterationAdaptiveDT
   [../]
#   dt = 2.e-3

   l_tol = 1e-2
   nl_max_its = 200
   nl_rel_tol = 1e-6
   nl_abs_tol = 1e-8

   solve_type = 'PJFNK'
   petsc_options_iname = '-pc_type -pc_hypre_type -
ksp_gmres_restart '
   petsc_options_value = 'hypre boomeramg 100'
[]


[Outputs]
  file_base = c5g7-td0.1
  exodus = false
  csv = true
[]
```