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Simulation of TREAT Cores Using High-fidelity Neutronics Code PROTEUS

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Abstract - *Two TREAT experimental cores, Minimum Critical Core (MinCC) and M8CAL, were simulated for verification and validation tests of PROTEUS. Due to the significant neutron streaming effect in the test problems via air cooling channels and hodoscope slot, the MOCEX solver of PROTEUS was used for the simulation. For systematic verification tests, 2D and 3D single fuel element, partial core, and whole-core problems were constructed and simulated, aiming at 3D whole-core calculations with explicit geometry configurations. Meshes were generated using the PROTEUS mesh toolkit combined with CUBIT. Multigroup cross sections were generated from the Serpent Monte Carlo code based on the 11 energy group structure to focus on the verification of the transport solution accuracy of PROTEUS. The simulation results for various cases based on MinCC and M8CAL indicated that the PROTEUS eigenvalues and power distributions were in very good agreement with Serpent solutions.*

I. INTRODUCTION

The PROTEUS code is a high-fidelity three-dimensional (3D) deterministic neutron transport code developed by Argonne National Laboratory (ANL) under the Department of Energy, Nuclear Energy Advanced Modeling and Simulation (DOE NEAMS) program. [1] The code contains the SN2ND [2] (second order discrete ordinates method) and two MOC transport solvers, MOCFE and MOCEX [3] (first order methods of characteristics), based on unstructured finite element meshes, allowing users to model complex or unconventional geometry reactor problems. Among the two MOC solvers which normally perform better than S_N for heterogeneous geometry problems, MOCEX is based on a rigorous formulation using two-dimensional (2D) MOC radially and the discontinuous Galerkin finite element method axially to overcome the drawbacks of MOCFE with the full 3D MOC representation requiring enormous memory and computational effort.

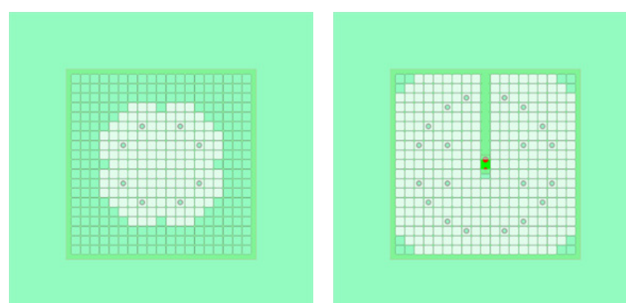
As a code verification and validation effort, PROTEUS has been used to simulate the Transient Reactor Test Facility (TREAT) [4] which is an experimental reactor designed for the testing of nuclear fuels and other materials under transient conditions. Due to the air cooling channels of TREAT, the MOCEX solver is used to accurately simulate a full 3D heterogeneous geometry model of two experiment configurations of TREAT. Results of these simulations are provided in this paper.

II. TREAT MODELS FOR PROTEUS

1. Simulation Models

TREAT is a heterogeneous, air-cooled, graphite-moderated and graphite-reflected thermal reactor. A detailed description of TREAT can be found in the facility's 1960 design summary report [4]. The reactor is fueled with highly-enriched (~93%) UO_2 dispersed in graphite, with a fuel carbon-to-uranium (C/U) atomic ratio of roughly 10,000 to 1. The fuel is arranged in zircaloy-clad fuel elements, with an approximately 4 ft long central fuel section and 2 ft long aluminum-clad graphite reflectors above and below the fuel. The elements are approximately 4 in x 4 in square, with chamfered corners. The reactor core can accommodate a maximum of 361 elements, arranged in a 19x19 array and surrounded by a permanent graphite reflector. The experiment vehicles for sample irradiation were placed at the center of the core, and typically replaced 1-4 fuel elements. Sample behavior during a transient was monitored by an ex-core system of collimated detectors called hodoscope. A partial ("half-slotted") or full ("full-slotted) row of central fuel elements was often removed to provide an unimpeded path for neutrons between the experiment and hodoscope.

Current modeling and simulation of TREAT are challenging due to long-standing uncertainties in core properties, including the boron and iron impurity contents and graphitized-to-total carbon ratio of the TREAT fuel, and limitations in the currently-available historic measured data.



MinCC M8CAL

Fig. 1. MinCC and M8CAL of TREAT

In this study, we selected two experiment models for PROTEUS simulation, the Minimum Critical Core (MinCC) and the half-slotted M8CAL core, as shown in Fig. 1, with the following assumed core conditions: 7.53 ppm boron and 267 ppm iron impurity in the graphite fuel, 59%

graphitization, 16 zircaloy-clad dummy elements for MinCC, and heated condition at 294K. Core eigenvalues resulted from the Serpent Monte Carlo code [5] with the ENDF/B-VII.1 MCNP library are 1.00490 ± 0.00019 and 1.00394 ± 0.00020 for MinCC and M8CAL, respectively. [6] All control rods are out for MinCC, while control rods are partially inserted for M8CAL.

Significant neutron streaming through air cooling channels of element's chamfered corners and hodoscope slot is challenging for deterministic codes. However, the 3D formulation of MOCEX based on 2D MOC along with the discontinuous Galerkin finite element method axially, represented as Eqs. (1) and (2), is capable of accurately simulating such neutronics challenge.

$$\varphi_i(x,y,z,\Omega) \approx \sum_{j=1}^{N} \varphi_i^j(x,y,\Omega)u_i^j(z) , \tag{1}$$

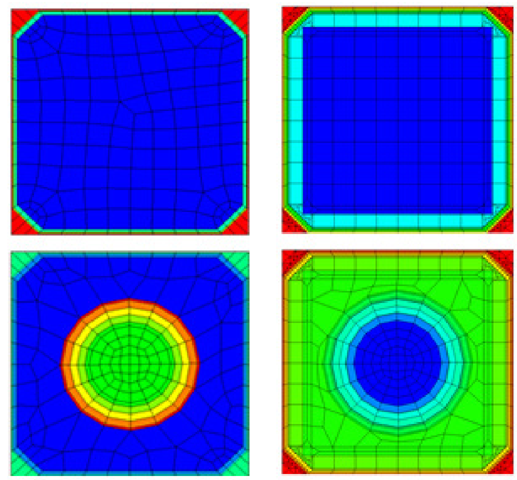
$$q_i(x,y,z,\Omega) \approx \sum_{j=1}^{N} q_i^j(x,y,\Omega)u_i^j(z) , \tag{2}$$

where φ_i and q_i are the neutron flux and source for a 3D mesh i, respectively, and $u_i^j(z)$ is the j-th basis function.

2. Mesh Generation

For PROTEUS calculations with MOCEX, meshes were generated using the meshing toolkit [7] of the PROTEUS package combined with the CUBIT mesh generation software [8]. Meshes for standard hexagonal or Cartesian types can be generated using the PROTEUS meshing tool alone, but components with complex or irregular geometries are generated using CUBIT and then are merged together using the PROTEUS meshing tool. For TREAT, the fuel, control rod, and zirconium-clad or aluminum-clad dummy elements with chamfered corners were modeled and meshed using CUBIT. These were then merged together to construct partial- or whole-core problems using the PROTEUS meshing tool. The meshes for the permanent graphite reflector (PGR), as well as the air gap between the core and PGR, were also generated using the PROTEUS meshing toolkit. Since it is based on the extruded geometry formulation, MOCEX requires 2D projected meshes only with which 3D geometry representation is given via a user input.

The meshes used for fuel and control rod element components are shown in Fig. 2. The normal mesh was generated for initial verification tests of simple geometry models, but later on the 2D projected meshes were generated to simulate actual 3D cores with axially non-uniform geometries. For example, the normal meshes include only 4 regions for the fuel element and only 9 regions for the control rod element, while the 2D projected meshes are composed of 8 regions for the fuel element and 17 regions for the control rod element. In particular, the experiment vehicle located at the core center of M8CAL was separately generated in a three-element size and merged to complete the 3D whole-core M8CAL mesh. The hodoscope channel in the permanent graphite block was separately defined and merged as well. As aforementioned, the graphite blocks above and below the hodoscope channel were represented using an additional input file containing the mapping between geometry and composition. Figures 3 and 4 show 2D whole-core meshes for MinCC and M8CAL, respectively.



(Normal Mesh) (2D Projected Mesh)
Fig. 2. Fuel and Control Element Meshes for PROTEUS.

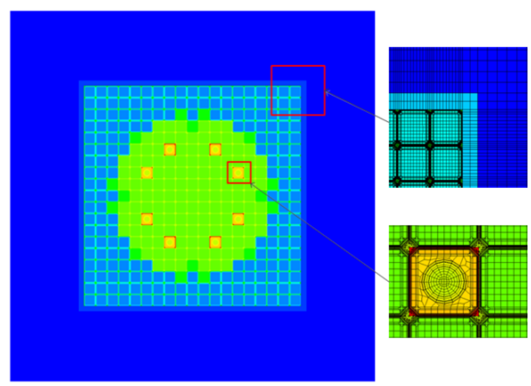


Fig. 3. 2D Projected Core Mesh of MinCC.

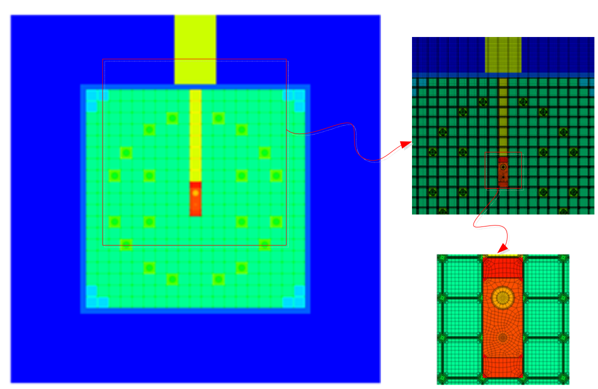


Fig 4. 2D Projected Core Mesh of M8CAL.

3. Multigroup Cross Section Generation

In this study, macroscopic cross sections were generated using Serpent to focus on verification of the transport solution accuracy of MOCEX. An 11 energy group structure was determined based on preliminary studies, starting from the 23 energy group structure used for VHTR analysis [9] and making a group optimization effort to reduce the number of energy groups maintaining most of the accuracy of the 23 group solutions. The GenISOTXS code [10], which was developed by ANL to process cross sections generated from Serpent or OpenMC Monte Carlo codes, was used to verify macroscopic cross sections from Serpent and to convert them to the ISOTXS format readable by PROTEUS.

The lethargies of the 11-group structure are depicted in Fig. 5, in which the 9-group structure traditionally used for graphite-moderator cores are compared as well. In the 11-group structure, small energy intervals are given in the energy range of 0.2 - 4 eV and around 1 MeV. Cross sections for different compositions were generated for each element type to reduce the number of cross section sets necessary for PROTEUS calculations (although they should be generated for each region with different material, location, and number density considering correct resonance self-shielding and neutron spectrum effects). Preliminary analysis indicated that generating composition-wise cross sections for each element type along with 11 groups did not affect solution accuracy significantly. Since an accuracy issue was found in the high-order scattering moments generated from Serpent, the transport approximation approach was used, in which total cross sections and within-group scattering cross sections were adjusted by the total P_1 scattering cross sections. It was observed that eigenvalue solutions were increased by ~100 pcm with P_2 scattering cross sections generated from Serpent and there were almost no differences between solutions with P_2 and P_3 scattering cross sections.

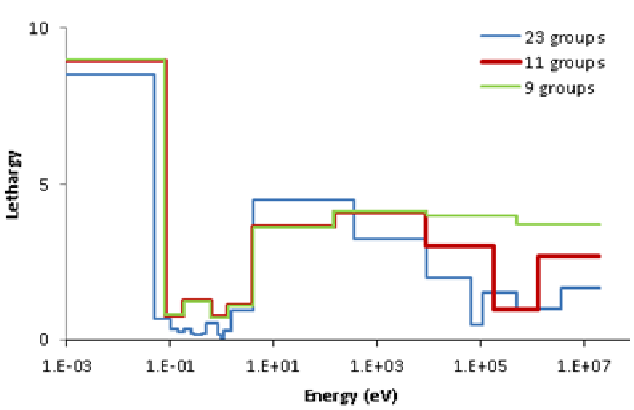


Fig. 5. Group Structures Used in PROTEUS for TREAT.

III. VERIFICATION RESULTS

For systematic verification tests, benchmark models were created based on the actual MinCC and M8CAL models, which include a single fuel element, a 2D core with or without PGR, a 3D single fuel element, and a 3D partial core. The 2D core is composed of 133 fuel elements, 8 control rod elements, and 16 zircaloy-clad and 204 aluminum-clad dummy graphite reflector elements in the core region. A reflective boundary condition is applied to the 2D core without PGR, whereas a vacuum boundary condition is used for the one with PGR.

Table I shows eigenvalue comparison between PROTEUS-MOCEX and Serpent. Most of the PROTEUS calculations used a Legendre (polar) Tchebychev (azimuthal) cubature order of L5T15 (192 directions on a sphere), 11 energy groups, and 0.05 cm ray spacing. A full domain decomposition was performed in terms of angle and space, except for energy. As shown in Table I, 2D cases including a single fuel element and 2D cores with or without PGR showed good agreement in eigenvalue between PROTEUS and Serpent.

Table I. Eigenvalues of MinCC and M8CAL cases from PROTEUS and Serpent.

Case		Serpent	PROTEUS	
			Angle	Δk, pcm
2D Fuel Element		1.66673 ± 3 [d]		-32
MinCC	2D Core w/o PGR [a]	1.29939 ± 15	L5T15	15
	2D Core w/ PGR	1.23041 ± 22		-213
	3D Single FE [b]	1.45473 ± 20	L5T15 L15T15 L15T25	214 158 140
	3D 2x2 (3FE,1CE)	1.27926 ± 21	L5T15 L15T15 L15T25	149 69 43
	3D 2x2 (2FE,2CE)	1.16952 ± 21	L5T15 L15T15 L15T25	18 -72 -98
	3D Full Core	1.00490 ± 19	L5T15	-1
M8CAL	3D Partial Core	1.37609 ± 16	L5T15 L15T15 L15T25	249 207 186
	3D Full Core [c]	1.00497 ± 18	L5T15	66

a) PGR: permanent graphite reflector; b) FE: fuel element; c) Simplified model; d) standard deviation, pcm.

PROTEUS flux solutions for the 2D MinCC core with PGR are illustrated in Fig. 6. Even with air channels, 2D cases are relatively easier than 3D to solve because neutrons move in the radial direction only and furthermore the air channels are geometrically symmetric.

The 3D MinCC is composed of 26 distinct axial layers with different geometry or compositions. Due to the geometric complexity of the actual core, a few complex geometries at thin axial layers right above and below the fuel element were homogenized, which have little effect on solution accuracy. In the PROTEUS calculations, 42 planes were assigned axially with less than 10-12 cm per axial plane, resulting in 12 planes for the fuel region of ~120 cm high in the middle of the core.

Prior to the 3D whole-core calculation for MinCC, a 3D single-element case with top and bottom graphite reflectors was analyzed. A vacuum boundary condition was applied to the top and bottom ends. From preliminary analysis [11] with homogeneous and heterogeneous geometry models, it was found that the neutron streaming effect through the air cooling channel is up to 700 pcm.

The PROTEUS calculation for the 3D fuel element model with the explicit geometry resulted in a good estimation of eigenvalue, which agreed with the Serpent solution within 140 pcm when a sufficient order of angular quadrature was given, especially for the polar direction due to the air channels.

Two 3D 2x2 element models, using 3 fuel and 1 control rod elements or 2 fuel and 2 control rod elements in a checker board pattern, were constructed and tested to ensure that the 3D geometry and composition assignments were correct for both fuel and control rod elements. As shown in Table I, the PROTEUS eigenvalues are in good agreement with the Serpent results within 98 pcm.

Based on the 2D mesh shown in Fig. 3, finally, a 3D full-core MinCC was calculated using PROTEUS as well, resulting in excellent agreement in eigenvalue with Serpent. Figure 6 shows thermal and fast neutron flux distributions of 2D MinCC.

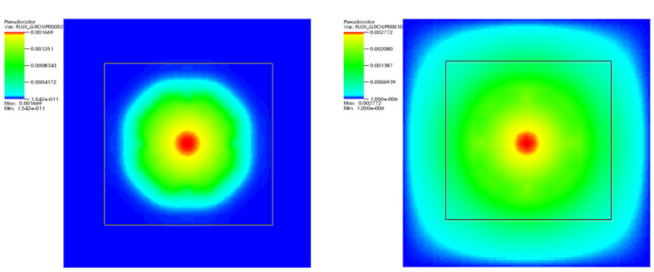
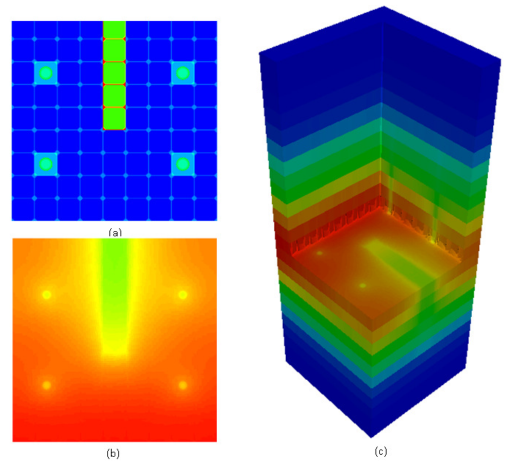


Fig. 6. Fast (left) and Thermal (right) Flux Solutions of PROTEUS for 2D MinCC.

For deterministic codes, M8CAL is neutronically more challenging than MinCC because of its large hodoscope air channel. Prior to a 3D whole-core calculation of M8CAL, a small 3D problem with 9x9 elements including 72 fuel elements, 4 control rod elements, and 5-element-size air channel was constructed, maintaining the axial configuration of the 3D whole core case and excluding the experiment vehicle in the core center.

In Table I, the eigenvalue results from PROTEUS and Serpent calculations show good agreement. The difference of 249 pcm with an angular cubature order of L5T15 was further reduced to 186 pcm by using the finer angle L15T25 as expected. Fast group flux solutions for 2D and 3D slices of the problem are illustrated in Fig. 7, showing the neutron streaming effect on the hodoscope slot.



(a) Loading, (b) 2D Fast Flux, (c) 3D Fast Flux

Fig. 7. Core configuration and 2D and 3D Fast Flux Solutions of PROTEUS for Small 3D M8CAL

Based on the 2D mesh shown in Fig. 4, a 3D full-core M8CAL model, simpler than the actual M8CAL experiment, was constructed excluding the experiment vehicle and simplifying geometry and composition axially. The control rods were inserted to make eigenvalue of the simplified model become 1.00497: 8 control/shutdown control rods were inserted deeply by 91.5 cm, 8 transient control rods were located to 48.7 cm from the top, and 4 compensation/shutdown control rods were out of the core. The hodoscope air channel in the permanent graphite block is 48.4 cm wide and 121 cm high, as shown in Fig. 8.

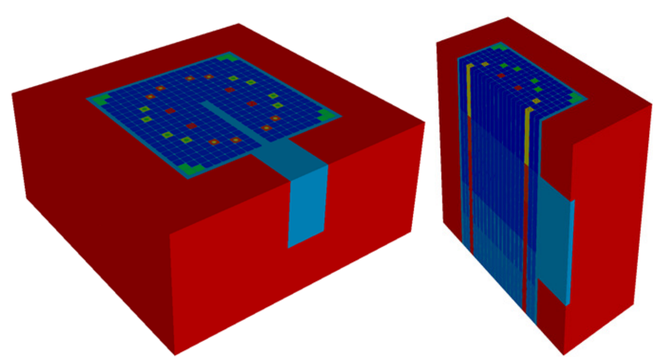


Fig. 8. Core configuration of Full 3D M8CAL (Simplified Model).

The eigenvalue solution of PROTEUS agreed very well with the Serpent solution within 66 pcm. The fast and thermal neutron flux distributions from PROTEUS are illustrated in Fig. 9, showing a significant neutron streaming through the hodoscope channel. This indicates that an accurate estimation of the neutron stream effect to the hodoscope channel is very important for this problem.

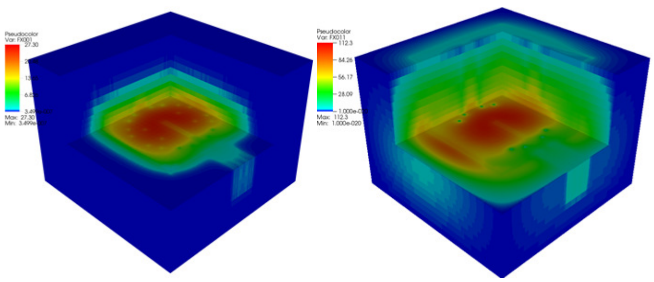


Fig. 9. 3D Fast (left) and Thermal (right) Flux Solutions of PROTEUS for Full 3D M8CAL.

For more detailed verification, axially integrated power distributions were compared between Serpent and PROTEUS. MinCC is 1/8-th symmetric and has no control rods inserted. Power distributions are smoothly varying with depressions (relative power: 0.7) at the control rod locations. Therefore, PROTEUS and Serpent solutions agreed excellently within maximum difference of 0.44% and RMS difference of 0.22%. Since most of the large errors come from the outmost fuel elements, differences are down to maximum difference of 0.30% and RMS difference of 0.14% if excluding the outmost fuel elements.

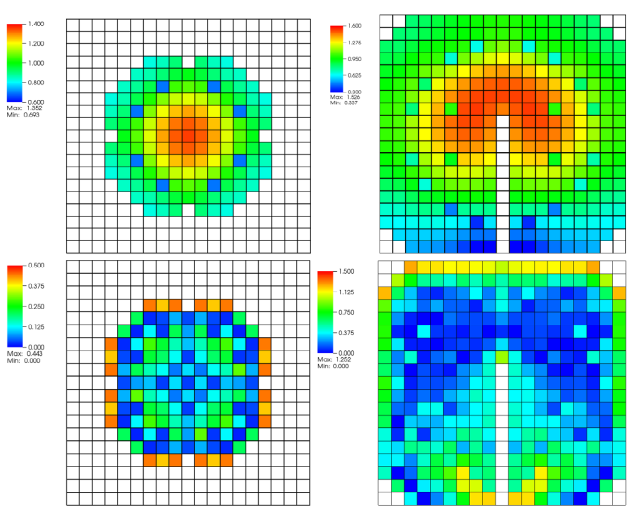


Fig. 10. Axially Integrated Fuel Element Power (top row) and Percent Difference (bottom row) Distributions for MinCC (Max: 0.44%, RMS: 0.22%) and M8CAL (Max: 1.25%, RMS: 0.50%).

Power distributions of M8CAL vary significantly with locations due to control rods inserted and hodoscope air channel from the core center all the way to the outside of the core. The relative powers at the control rod locations and around the hodoscope channel are down to 0.3. Nevertheless, PROTEUS and Serpent solutions are in very good agreements within maximum difference of 1.25% and RMS difference of 0.50%. Excluding the outmost 3 fuel blocks, differences are down to maximum difference of 0.97% and RMS difference of 0.32%. Power and percent difference distributions for 3D MinCC and M8CAL are illustrated in Fig. 10.

IV. CONCLUSIONS

Two TREAT experimental cores, MinCC and M8CAL, were selected for code verification and validation test cases for PROTEUS. Due to the significant neutron streaming effect in the test problems via air cooling channels and hodoscope slot, the MOCEX solver of PROTEUS was used for the simulation. For systematic verification tests, 2D and 3D single fuel element, partial core, and whole-core problems were constructed and simulated using PROTEUS, aiming at 3D whole-core calculations with explicit geometry configurations. Meshes were generated using the PROTEUS mesh toolkit combined with CUBIT. Multigroup cross sections were generated from the Serpent Monte Carlo code based on the 11 energy group structure to focus on the verification of the transport solution accuracy of PROTEUS.

The simulation results for various cases based on MinCC and M8CAL indicated that the PROTEUS eigenvalues and power distributions were in good agreement with Serpent solutions, even with significant neutron streaming through air cooling channels or the large air channel to the hodoscope.

In future, the actual geometry and composition of M8CAL experiment will be modeled and simulated, including the experiment vehicle. In addition, instead of Serpent-generated cross sections, the cross section API inside PROTEUS will be tested for all the cases.

ACKNOWLEDGMENTS

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