Benchmark Evaluation of TREAT Reactor M2 and M3 Transient Experiments

Mission Supporting Transformative Research: Integral Benchmark Evaluations

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Project Title: BENCHMARK EVALUATION OF TREAT REACTOR M2 AND M3 TRANSIENT EXPERIMENTS

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Project Objective: The objective of this project is to evaluate and produce TREAT reactor benchmarks under steady state and transient conditions. The benchmarks support the TREAT restart effort and are to be contributed to the International Reactor Physics Experiment Evaluation Project (IRPhEP) for inclusion in the International Handbook of Evaluated Reactor Physics Benchmark Experiments. The benchmark evaluation is performed using data generated during the “Power Calibration Experiment for test M2” and “IFR Safety Tests M2 and M3”. The evaluations are conducted using the high fidelity Serpent-OpenFOAM code system. Both the steady state and transient conditions of the M2 and M3 tests were investigated. Furthermore, TREAT has a graphitic core. Historical work has shown that the predictions of the outcomes of TREAT tests are highly sensitive to the graphite thermal neutron scattering cross sections. Therefore, in this project, thermal neutron scattering (i.e., $S(\alpha,\beta)$) libraries of graphite, tailored to the specifics of the TREAT core, were generated and utilized in the evaluation.

Background: The Transient Reactor Test Facility (TREAT) has historically provided the capability for transient fuel performance and safety testing in the United States. The operation of this facility was suspended in 1994. However, in recent years preparations for the restart of TREAT were initiated. TREAT is a graphite moderated and air cooled reactor. Its core is composed of a 19×19 array of fuel assemblies that contain UO$_2$ (HEU) dispersed in a graphite matrix, along with reflector assemblies filled with graphite only. Each assembly is 8 feet tall with a fueled region that is 4 feet tall and upper and lower regions of graphite that are 2 feet tall. In addition, a 2 feet thick radial graphite reflector region is present. Finally, a 5 feet thick concrete biological shield surrounds the core.
Traditionally, experiments for fuel irradiation testing were performed in TREAT under steady state and transient conditions. As a primary test observable the power coupling factor (PCF), representing energy generated in the test fuel relative to the energy generated in the core, is quantified during low power level steady state fuel testing experiments (LLSS). Subsequently, a transient correction factor (TCF), estimated from prior calibration experiments (using wire samples), is applied to obtain the PCF throughout the transient test. In this project, the TREAT M2 calibration experiment and the M2 and M3 slow transient tests were evaluated and data extracted (e.g, effective multiplication factor (keff), PCF, TCF, test fuel axial power profiles, test fuel radial power profiles, test vehicle temperature data, etc.) to be used in benchmark analysis where the predictions of codes such as MCNP and Serpent for LLSS critical measurements. The validation of modern multi-physics computational tools for supporting TREAT restart and eventual utilization in advanced fuel testing campaigns represents a highly desirable contribution that would reduce the costly (time and funding) experimental overhead for conducting TREAT experiments.

The thermal neutron spectrum that develops during the operation of TREAT is highly affected by the phenomenon of thermalization in graphite. Previous work showed that the graphite thermal scattering cross sections can introduce variations exceeding 2000 pcm in the predicted eigenvalue of the TREAT core. In this project, TREAT specific thermal neutron scattering cross section libraries were prepared for use in Serpent for accurately simulating the M2 and M3 TREAT tests.

The outcome of this benchmark effort was contributed to the International Reactor Physics Experiment Evaluation Project (IRPhEP) for eventual inclusion in the International Handbook of Evaluated Reactor Physics Benchmark Experiments. The required IRPhEP procedures and formats were followed in conducting this evaluation. The contributed information included detailed descriptions of the M2 and M3 experiments and measured data, comprehensive evaluation of experimental parameters including assessment of unavailable information, provision of benchmark specifications, addressing known simplification biases (e.g., due to modeling approximations), provision of best-estimate sample calculations, and appendices with input codes and other supporting information.
1) TREAT Multi-Physics Simulations in support of benchmark analysis

TREAT is a high-enriched, homogeneous fueled reactor that is air-cooled, graphite moderated, and graphite reflected. This thermal spectrum reactor is dominated by a large temperature feedback coefficient and heat transfer properties from the graphite. The UO$_2$ fuel, enriched to 93.1wt%, is finely dispersed in a graphite matrix that provides a large thermal feedback safety mechanism as well as the ability to dissipate large amounts of heat from the fuel into the graphite.

The TREAT graphite has a density of 1.67g/cm$^3$ consistent with the density range of typical reactor grade graphite. This is compared with the much higher density of 2.25g/cm$^3$ for ideal graphite. This density difference is indicative of a structural difference between ideal graphite and reactor grade graphite. It has been theorized that the density and structural difference can be represented using a porous system and that a porous structure would impact thermal neutron scattering as a result of its higher cross section.

Figure 1 shows cross sectional views of the TREAT M2/M3 core configuration as constructed in the Serpent code. The experimental vehicle is located in the center of the core and the source element in the top right (north east) corner. The circles represent the control/transient rods, and the red regions correspond to the fuel. The fuel elements in TREAT are arranged in a 19 by 19 lattice with two concentric rings of control rods. Centrally located is the experimental vehicle hosting the test fuel or flux wire.

Fig. 1. (Top) TREAT cross sectional view of the M2/M3 core configuration as constructed in the Serpent model. The experimental vehicle is located in the center of the core and the source element in the top right (north east) corner. The circles represent the control/transient rods, and the red regions correspond to the fuel. (Bottom) Axial cross sections of the TREAT Serpent core geometry from north to south (right) and east to west (left). While the core elements were modeled in full detail, some approximations were introduced to simplify the graphite reflector.
Initially, steady state analysis was performed and compared to published experimental data sets for the M2/M3 experiments, which can be used to validate the models that were created. The steady state flux wire gives a full core axial power profile. The test pins provide axial power distributions at the experimental location as well as the absolute number of fissions in the test pins. The test pin distributions then contribute to the power coupling factor (PCF) which relates the fission density in the test pins to full core power. The third experimental data point used is the effective eigenvalue ($k_{eff}$) of the core model in the critical configuration and with critical rod heights.

Experimentally, the axial profiles from the flux wires and test fuel pins were determined from the gamma-ray counts which were then related to relative fission product activity per gram of fuel. Activity is directly proportional to fission rate so these results were replicated using energy deposition tallies. The results for these calculations for flux wire 48.1 are displayed in Fig. 2 with example results of the test pin (M2-3).

The flux wire distribution shows reasonable agreement with experimental data. The largest deviation occurs at the top third of the core. This effect is directly related to control rod height. The control rods were modeled at the specific critical heights reported in the reactor logs. However, those heights can contain up to ±0.02 inches error from indicated values with an additional 0.375 inches of uncertainty from the discrepancies in control rod diagrams. Lowering the rods further into the core, results in reduced relative activities at the top of the core only, giving slightly better agreement with the experimental data. The three fuel pins follow the same trend as displayed for the M2-3 pin. The shaping effect due to the dysprosium collar is clearly seen. The experimental and calculated values again show good agreement.

Using the flux profiles for the fuel pins, the PCF for the M2/M3 experiments was then calculated. PCF is defined to be

$$ PCF_{\text{experimental}} = \frac{fissions}{g_{\text{U-235}}} \cdot 27.2 \cdot \frac{pJ}{fission} \cdot \frac{\text{TREAT energy released}}{\text{TREAT energy released}}, $$

where $pJ$ is energy in pico jules. The power coupling factor is directly proportional to the fission density ratio for the core to fuel pins. Operators combined data from the core power monitors and the fission densities, determined from the fuel pin activities, to calculate the coupling factor. An additional 0.03W/gram per MW TREAT power was added to account for γ-heating and 1.6 MeV/fission to account for energy from β-decay. These results were replicated computationally with an additional component from the experimental data added to account for the β-decay. The resulting PCF values are displayed in Table I.

![Fig. 2. M2CAL flux wire 48.1 relative activity experimental (red) and calculated values (left). M2CAL test pin M2-3 relative activity experimental (red) and calculated values (right).](image-url)
Table I. Power Coupling Factor.

<table>
<thead>
<tr>
<th></th>
<th>Calculated (C)</th>
<th>Experiment (E)</th>
<th>C - E</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>PCF</td>
<td>Error (10%)</td>
<td></td>
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<tr>
<td>Pin 1</td>
<td>5.89 ±0.069</td>
<td>5.81 ±0.581</td>
<td>0.0134</td>
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<tr>
<td>Pin 2</td>
<td>6.06 ±0.071</td>
<td>5.99 ±0.599</td>
<td>0.0112</td>
</tr>
<tr>
<td>Pin 3</td>
<td>6.03 ±0.072</td>
<td>5.89 ±0.589</td>
<td>0.0233</td>
</tr>
<tr>
<td>Average</td>
<td>5.99 ±0.041</td>
<td>5.90 ±0.590</td>
<td>0.016</td>
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</table>

Transient operation for the M2 and M3 experiments began first with test wire irradiations, as described above, followed by the actual test pins. Transient 2580 was one such calibration transient conducted with a full-length, U-Zr flux wire in the experimental vehicle in the middle of the core. The transient lasted approximately 10 seconds from the initial rod withdrawal to shutdown, beginning in an initially critical state and 50W estimated power. The measured power data points along with experimental rod height are seen in Fig. 3. Prior to the transient, all control rods were fully withdrawn from the core with the transient rods T-1 reinserted 8.8 inches to maintain criticality. Transient rods T-2 were fully inserted in the critical configuration. The M2 and M3 transients began with an initial rod withdrawal for a step reactivity insertion establishing a stable period as power exponentially increased. For transient 2580, this rod withdrawal was the equivalent of 1110 pcm of reactivity insertion. The power rise was terminated with a combination of temperature feedback and rod reinsertion. Power was then leveled off and held constant for approximately 4 seconds to allow the system to pre-heat. After this time, the rods were further withdrawn from the core, ramping the power to higher levels until the rods reached a pre-programmed setpoint. In this test experiment, the rods were set to SCRAM upon reaching a certain height.

The average fuel temperature prior to the transient was measured to be 295K, and the maximum fuel temperature during the transient, sampled from 11 thermocouples in the core, was measured to be 354K. The TREAT graphite thermal scattering cross section is dependent on temperature with changes to the cross section driving feedback effects in the reactor. This is especially seen in Fig. 3 between 3.4 and 7.2 seconds where rods are steadily withdrawn yet power remains constant.

Fig. 3. Experimental power data points plotted with rod height as a function of time for M2 transient 2580 [10].

Serpent 2.1.29 is the Monte Carlo neutronics code used in this work. It has many capabilities such as determining the k-eigenvalue of a system and computing reaction rates using collision estimators. By including delayed neutron precursors and time-dependent neutrons, Serpent is able to simulate time-
dependent neutronic systems. Time-dependent simulations begin by defining the initial critical system to generate the source neutron and precursor distributions in space and time. This distribution represents time zero for the system and is used as the initial input for transient simulations. Transients are progressed through time in step increments.

Serpent is capable of reading material, geometry, and system properties from a variety of internal and external sources. In the coupled mode with an unstructured mesh, Serpent uses the traditional material and geometry definitions internally defined, but temperatures and densities of the specified materials are defined and updated from external calculations.

At the end of a time step, Serpent outputs neutronic parameters (e.g. reactor power), and the neutron population is normalized. The reactor power output by Serpent is calculated as the total fission energy deposition $\kappa \Sigma_f \phi$, where $\Sigma_f$ is the macroscopic fission cross section, $\phi$ is the neutron flux, and $\kappa$ is the heat deposited from fission. The default value of $\kappa$ for $^{235}\text{U}$ fission is 202.27 MeV with the heating value for other nuclides determined by the scaling of the ratio of fission Q-values. Properties of the system are then updated. For example, rod height which changes at a certain velocity will be moved to the next position at the end of a time step. In coupled mode, temperature is calculated externally, updated in Serpent at the end of a time step, and held constant over the time step. Temperature effects are treated within Serpent using an interpolation scheme for thermal bound scattering and an on-the-fly target motion sampling treatment for the free atom cross sections. Target motion sampling introduces Doppler broadening effects in the cross section by determining the thermal motion of the target nucleus by sampling a temperature-dependent Maxwell-Boltzmann velocity distribution.

Coupled to Serpent for the analysis performed in this work is the OpenFOAM 3.0.1 code. This is a finite volume, open source computational fluid dynamic code. The geometric domain is meshed into small volumes where the specified equations are solved with simple to implement tensor mechanics. In the case of the TREAT reactor, the fuel is solid with air cooling. However, the air channels are small and meshing these volumes to a reliable degree would increase the mesh size by several orders of magnitude. Instead, the current OpenFOAM model does not capture the cooling channels in the core. As implemented, the core in this model was considered a solid cube with the core elements coarsely meshed. This effectively assumes an adiabatic situation which given the short duration of the transient is considered a reasonable approximation. In order to determine the temperature of the fuel and conduct heat in the core, the time-dependent OpenFOAM “laplacianFoam” solver was modified to include a source term. The volumetric power from Serpent is applied as a constant source for the time step interval. The modified version of “laplacianFoam” then solved the following heat conduction equation

$$\frac{\partial T}{\partial t} - \frac{1}{\rho c_p} \nabla \cdot (k \nabla T) = \frac{q}{\rho c_p},$$

where $T$ is temperature [K], $k$ is thermal conductivity [W/m/K], $\rho$ is the density [kg/m$^3$], $c_p$ is specific heat [J/kg/K], and $q$ is the power output from Serpent [W/m$^3$]. OpenFOAM solves the heat conduction equation with Neumann (zeroGradient) boundary conditions. This boundary condition is applied to the edge of the core which is within the graphite region.

Serpent and OpenFOAM are linked through a file sharing system and a python script which iterates between the two codes as seen in Fig. 4. Serpent communicates with external solvers through output and input files. By separating the state point properties of the reactor to OpenFOAM, temperature distributions across a fine mesh can be applied to a complex geometry. Combined with the on-the-fly target motion sampling (TMS) for temperature treatment of the free atom cross section libraries and on-the-fly interpolation for the thermal scattering libraries, temperature related effects across the domain can be coupled into advanced neutronic calculations.

In coupled calculations, Serpent outputs the integral fission power for each mesh volume at the end of every time interval on the same mesh read by OpenFOAM. Once Serpent has produced the power mesh for a time step, Serpent calculations are paused while temperatures are calculated. OpenFOAM then uses this
source term in a modified version of the “laplacianFoam” solver to generate temperature distributions across the mesh corresponding to the end of the Serpent time interval. Sufficiently small time steps are required to accurately coordinate the power and derived temperatures. The current model for TREAT only calculates temperature; however, given the flexibility of the Serpent-OpenFOAM system, densities can also be determined and applied to the Serpent calculation. This is not needed for a solid fuel system during a short transient. Once the temperature calculations are complete, the python script signals Serpent to continue to the next time step. During this new time step and for each interaction, Serpent uses an adaptive search mesh algorithm to comb through the OpenFOAM mesh to determine the correct temperature for the material in the interaction. Based on this temperature, the on-the-fly routines adjust the cross sections.

![Flow chart of coupled Serpent-OpenFOAM system](image)

**Fig. 4. Flow chart of coupled Serpent-OpenFOAM system. Using the parameters defined in Serpent and OpenFOAM, a coupling script uses the algorithm described here to relay information between codes to result in a coupled, multi-physics system.**

The developed Serpent model and described above served as the basis of the steady state and transient benchmark analysis of this project. Transient 2580 was known to start from a critical configuration which allows Serpent’s assumptions for the initial conditions to hold true. TREAT fuel is contaminated with various impurities, the most significant being boron. The average boron concentration is estimated to range between 5.9 ppm to 7.6 ppm. By adjusting the boron concentration in the graphite fuel matrix throughout the core the system was made critical. This adjustment of the boron concentration is indicative of other potential uncertainties in components affecting reactivity in TREAT. For example, it has been previously noted that modified graphite thermal cross sections are needed in order to properly represent the reactor graphite in a system like TREAT. Using this critical configuration, the initial distribution for the steady state neutron population was calculated using 80,000 particles over 5,200 cycles with an additional 200 cycles skipped which was verified to result in fission source convergence. The initial critical system was calculated to have a $k_{eff}$ of 1.00017 ± 0.00005, and the resulting power tallies in each mesh cell have an uncertainty less than 0.3%. The power maneuver and the M2 experiment was then initiated by ejecting the T-2 transient rods from the core.

For reactors such as TREAT, variations in reactivity are impacted by control rod movement and modifications to the neutron leakage rate as the temperature of the core’s graphite-fuel system varies. To predictively capture these effects, the Serpent-OpenFOAM system described above was used to calculate the time-dependent power maneuver from low power to 27MW for transient 2580. Transient simulations
for the coupled system proceeded as described above in Section 3.3. Temperature, rod position, and power were updated every 0.05 seconds. The initial neutron population in Serpent was normalized to 32W, which showed reasonable agreement with the experimental data. Further assessment of the value of initial power could be made and may improve the achieved level of agreement. For the first 3.5 seconds of the simulation, 1,000,000 initial source particle histories were tracked using time intervals of 0.05 seconds. After 3.5 seconds, 2,000,000 initial source particles were used every 0.05 seconds. Because of the rapid change of key reactivity components, additional precision was required after the initial 3.5 seconds, hence the larger number of particle histories. This provided a more precise power estimate which is then transferred to the OpenFOAM temperature calculation during the timeframes when rod position and temperature are concurrently changing.

The model used the reported rod heights for the rod withdrawal. However, it was found in the model that the positive reactivity insertion (due to rod withdrawal) was 1127±9pcm as compared with the 1110pcm experimental estimate. Therefore, during the rod maneuvers, the transient rods T-2 were inserted approximately 2 cm further into the core to compensate for the excessive initial positive reactivity. For the steady state region between 3.5sec and 7sec (see Fig. 3), the rod positions in the simulation were set to reproduce the reactor’s experimentally observed steady state critical behavior. The final transient power ramp was initiated within the model with a linear rod withdrawal rate resulting in a positive reactivity insertion to counter that of the temperature feedback.

Temperature distributions generated in OpenFOAM were calculated for a mesh with 14 axial slices, 12 of which being in the fuel region. In the X-Y direction, each element was meshed into a single square. This results in a mesh element size of approximately 10x10x10cm. An additional 4 inches of the reflector graphite on the top, bottom, and sides was included in the mesh. However, no heat was generated or transferred to this graphite. All temperature boundary conditions were defined such that the boundary temperature equals the temperature of the volume which it bounds (Neumann zeroGradient boundary conditions). Temperatures were only calculated for the graphite fuel matrix and were applied using the on-the-fly Serpent routines to account for variations in the neutron cross sections due to the Doppler effect in the fuel and thermal neutron scattering effects in the graphite moderator. All other material temperatures were held at 295K, which is expected to have minimal impact on the results of the simulation. In addition, to account for the difference in volume of the fueled region between OpenFOAM and Serpent, volume averaged values for the density (1.52 g/cm³), thermal conductivity (19.7W/m/K), and specific heat (707.2J/kg/K) were used in OpenFOAM. Notice that the used values are very close to the values for the fueled region in a TREAT element and are consistent with the fact the air gap represents a small fraction of the fuel element’s volume. These values were held constant and were not temperature dependent in the simulation. The OpenFOAM case used Euler’s method with linear interpolation and Gaussian integration schemes to determine the temperatures across the core. Time steps within OpenFOAM corresponded to those in Serpent. However, within the time-dependent OpenFOAM calculation, the temperature calculation was executed using 0.001 second intervals until the total time interval of 0.05 seconds was reached.

Iterating between neutronic analysis and generation of core temperatures for each time step, power and temperature as a function of time were calculated. Using hybrid distributed and shared memory compilation bindings (MPI and OpenMP) with 5 nodes and 28 processes per node (Intel Xenon x64 processors with a CPU clock speed of 3.2 GHz), 0.5 seconds of the transient was completed in approximately 4 hours wall time and used approximately 35GB of memory per MPI process depending on the code execution phase. The calculated flux was used to determine power as a function of time as shown in Fig. 5. The power data corresponds to the tally for fission energy production as a function of time, normalized to the experimental data in Fig. 6. The resulting temperature distribution of the graphite-fuel matrix takes the form seen in Fig. 7, which displays the temperature throughout the time of the simulation. The core averaged and core maximum fuel temperatures are given in Fig. 8.

Within the first second of the transient, a stable reactor period is established as power exponentially increases with no temperature feedback effects. Experimentally, this period was estimated to be 0.214±0.012 seconds. The model produces a period of 0.200±0.007 seconds calculated from the power between 2.05 seconds to 2.50 seconds as in the measurement. The volume averaged core temperature in
Fig. 8. follows the same trends noted in previous transients where temperature was monitored as a function of time. Specifically, the core temperature rise does not initiate until approximately 2 seconds after the initial rod ejection. By 2.5 seconds, temperature from the model is linearly increasing. The resulting temperature feedback combined with negative reactivity due to partial rod insertion at 2.65 seconds terminates the power increase and levels power off, resulting in an initial power peak. Experimentally, the initial power peak measurements ranged from 29.3MW to 31.6MW depending on the detector. A calculated value of 33.5MW is reached, which is somewhat higher but in reasonable agreement with the experiment.

Between approximately 3.5 to 7.0 seconds, rods are continuously withdrawn from the core. During this time, the calculated average core temperature continues to increase driving feedback effects and resulting in a constant power flattop as seen in Fig. 5. The transient ramp then begins around 7.0 seconds where positive reactivity contributions from rod withdrawal combine with negative reactivity effects from the increasing temperature to result in the linear power ramp. The model predicted rate of power increase was calculated to be 3.2MW/sec as compared with an average experimental value of 2.9MW/sec. This transient then results in a final temperature of 363.0K at the thermocouple location compared to the experimental value of 354K.

![Graph](image1)

**Fig. 5.** Absolute power calculations. The calculated power is compared with the experimental data on both linear-linear (left) and log-linear plots (right).

![Graph](image2)

**Fig. 6.** Core power maneuver. The calculated power is compared with the normalized experimental data for transient 2580 during the power increase and then for the initiation of the transient ramp.
Fig. 7. Core fuel temperature distributions plotted at the fuel centerline. The OpenFOAM temperatures for the fuel mesh are displayed at varied times throughout the simulation. The core averaged temperatures ($T_{avg}$) are also given at each time.

Fig. 8. Core average and core maximum fuel temperatures as calculated by the Serpent-OpenFOAM system.

TREAT MAMMOTH transients were executed based on a coupling between the Sn code RATTLESNAKE and the heat transfer code BISON. These methods require several initial inputs including
geometry and cross sections. The development of cross sections begins in the Monte Carlo code Serpent 2. Serpent allows for the generation of group cross sections and tallying of fluxes across a given universe. However as a Monte Carlo code, results are bounded with a statistical uncertainty such that materials further from the core see fewer particles and therefore have higher error. Additionally, the process of generating group cross sections is extremely time intensive in Serpent further contributing to the large amounts of computational power needed to tally cross sections for every single assembly. Previously, the solution was to group many assemblies together in order to calculate a single cross section with improved statistics. However, a single flux distribution was also calculated for that group of assemblies. The results was a still computationally intensive process with too few particles for good statistics in areas surrounding the core.

The proposed solution for the ex-core structures was to homogenize the optically thin regions of the core with some of the surrounding material in order to increase the interaction probability. For example, there is a 2 in air gap surrounding the core. This air gap along with a thin aluminum liner was homogenized with some of the graphite reflector in order to create one cross section. The same ideology was applied to the hodoscope slot and the detector slots around the core. This results in the geometry differences between the exact Serpent model and the homogenized MAMMOTH mesh that can be seen in Fig. 9.

![Fig. 9. TREAT core (top down view) for the M2CAL experiments in the Serpent code (left) and MAMMOTH (right). Red represents the fuel experiments, the circles in the Serpent model are the control rods. For the M2 experiment, the core is fully slotted north to south. To the north is the hodoscope slot along with detector holes to the north, south, and west in the radial graphite reflector.](image)

Comparing the cross sections from individual assemblies, it was found that fuel assembly cross sections deviate across the core by less than 3% which is well within the Monte Carlo error for the cross sections. This difference decreases with improved statistics. The only variation between assemblies is the flux. Given the material composition of TREAT, homogenization of the fuel with graphite along with the thermalization properties of graphite result in a consistent energy spectrum across the core. Additionally, the boron absorber in the control rods is also a 1/v absorber in the thermal region, again not causing shifts in the energy spectrum. This allows for cross sections across the core to be tallied in a single grouping. Because all the fuel assemblies are grouped for a single average cross section, statistics are vastly improved and computation time is reduced. Further, flux tallies can be defined across the core. Flux tallies allow for more precise representation of the flux across the core with more axial regions.

Using this theory, two models were created: one using the traditional method of many groups and one using only four cross section groups with many flux tallies, both of which are displayed in Fig. 10. The reduction in cross section groupings significantly decreases the run time such that nearly double the number of particles may be run for improved statistical errors in the fluxes.

Using group cross sections from Serpent, MAMMOTH was used to perform a Larsen-Trahan transport calculation (source problem) in order to obtain transport-corrected directional diffusion coefficients (TDC). A super homogenization (SPH) correction was applied to preserve the reaction rates given the fluxes in a region. These final cross sections were then used for a full-core diffusion calculation of power. Comparing the power distribution across axial slices of the core, much improvement is seen in the model with fewer
cross section groups. Using the full cross section method, errors in the power were in excess of 30% near the hodoscope even with the corrected diffusion coefficients. However, with the reduced model, the maximum error is 4.6% at the control rod location where separate flux tallies were not used. This error can be reduced even further if the method of applying flux tallies was also applied to the control rod assemblies.

Fig. 10. Initial full model (left) and final reduced model (right) for Serpent cross section generation in the core. Each color represents a different cross section zone. Initially, the core was split into 23 zones with each zone then further split into 19 axial slices. The reduced model has only 4 cross section zones with 19 axial slices. Fluxes were tallied for all 325 fuel assemblies with 19 axial slices in the reduced model.

Fig. 11. Error from a comparison of power density from Serpent and MAMMOTH in the fuel assemblies in the middle of the fuel using cross section with both TDC and SPH corrections. The initial full model (left) has large errors near the hodoscope region along with compensation effects at the bottom of the core. The final reduced model (right) shows much improvement with the largest errors in the control rod assemblies where the flux method was not applied.

Further, comparing the reaction rates in the core we see the same trend where the generation rate, absorption rate, source rate, and total flux all agree well between the two codes. A difference of approximately 3,000 pcm is seen between the eigenvalues, but this deviation is consistent with other results from MAMMOTH (Table 2). This method significantly reduces Serpent computational resources required for generating a single set of cross section data. Multiple points are required for a transient simulation, and this method will help ease the computation expense for accurate shaped transients in MAMMOTH. Flux
tallies across the core increase the fidelity of the SPH correction since each assembly now has accurate fluxes. Future work will apply these principles to a reduced core size. By representing a smaller block of assemblies rather than a full core, cross sections can be tabulated for changing rod heights without full core analysis.

Table 2. Comparison of eigenvalue and related components between MAMMOTH and Serpent.

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<th>Serpent</th>
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<th>MAMMOTH Reduced Model</th>
<th>% Diff.</th>
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<td>Generation Rate</td>
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<td>0.00%</td>
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<tr>
<td>Absorption Rate</td>
<td>7.09E+10</td>
<td>7.12E+10</td>
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<tr>
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</table>

2) Thermal neutron scattering and impact on TREAT

As previously noted, graphite thermal scattering is a vital component to successfully representing the moderation and thermalization physics of the TREAT reactor and its reactivity feedback behavior. Therefore, the impact of the graphite thermal neutron scattering cross section (as derived from the scattering law, S(α,β)) on the TREAT system should be considered. The density of the TREAT graphite corresponds to that of reactor graphite which has a different microstructure as compared with ideal graphite. This structural difference between ideal and reactor graphite has been represented as porosity in reactor graphite cross sections that were included in the ENDF/B-VIII.0 database. The 30% porous libraries are representative of the TREAT system given the density of the TREAT graphite. Comparing the ENDF/B-VII.1 and the reactor graphite cross section in ENDF/B-VIII.0 in Fig. 12, significant improvement in the cross sections is seen relative to experimental data. The expected deviation between the calculated and measured cross sections is due to temperature differences (i.e., 500K in the ENDF/B-VIII.0 library versus 478K in the measurement).

As seen in Fig. 12, the introduction of porosity increases the cross section. Implementing the two cross section libraries for a critical core configuration of TREAT, the predicted k_{eff} values are seen in Table 3. Reactor graphite cross sections result in an increase of 800pcm as compared to the ideal graphite case. In the comparison case here, a boron concentration of 7.53ppm is used based on the available historical data, corresponding to the average boron impurity for TREAT. Boron along with other contaminants within the TREAT fuel introduce large amounts of uncertainty in the modeling of the TREAT system. However, the contributions of the graphite thermal scattering library demonstrate significant improvement to the representation of the critical state. Using the ENDF/B-VII.1 cross sections, the core is significantly subcritical; however, with the use of the reactor graphite cross sections, the model predicts a significantly higher criticality level.

In addition, the reactivity impact of the different graphite thermal scattering libraries may be examined in terms of thermal spectral shifts. Figure 13 shows the calculated thermal flux spectra in the core at room temperature (initial transient temperature) and at 400K (representing maximum transient temperature). Based on this data, the average thermal neutron energy was determined, for ENDF/B-VII.1 graphite, to be 0.0935eV at 296K and 0.1029eV at 400K. For reactor graphite, the average energy is 0.0890eV at 296K
and 0.0997eV at 400K. The statistical uncertainty in the average energy is estimated to be ±0.0005eV, which indicates that the observed decrease in the average energy is representative of a down spectral shift to lower energies as a result of the enhanced thermalization expected from the ENDF/B-VIII.0 data. This correlates directly with the observation of an increase in $k_{\text{eff}}$ as a result of using the ENDF/B-VIII.0 thermal scattering cross section libraries. Similarly, Fig. 14 shows the leakage spectra.

Such changes to the spectrum would be expected to impact both the steady state and transient behavior of the reactor as observed and/or predicted using detector responses and quantities such as the power coupling factor (PCF) and the transient correction factor (TCF). Experimental estimation of these key core indicators relies on instrumentation located either in or beyond the core’s graphite reflector. Other factors of interest such as the incoming flux and spectral effects at the experiment location should also be impacted.

![Graphite total thermal scattering cross sections for ENDF/B-VII.1 and ENDF/B-VIII.0 reactor graphite (30% porous) with experimental data for reactor graphite.](image)

**Fig. 12.** Graphite total thermal scattering cross sections for ENDF/B-VII.1 and ENDF/B-VIII.0 reactor graphite (30% porous) with experimental data for reactor graphite.

**Table 3.** Reactivity differences from ENDF/B-VII.1 ideal graphite and ENDF/B-VIII.0 reactor graphite (30% porous). $k_{\text{eff}}$ Monte Carlo uncertainties were calculated to be ±7 pcm.

<table>
<thead>
<tr>
<th></th>
<th>$k_{\text{eff}}$ (296K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF/B-VII.1</td>
<td>0.98995</td>
</tr>
<tr>
<td>ENDF/B-VIII.0 (Reactor Graphite)</td>
<td>0.99785</td>
</tr>
<tr>
<td>Reactivity Difference (ENDF/B-VIII.0 − ENDF/B-VII.1)</td>
<td>+800 pcm</td>
</tr>
</tbody>
</table>
Fig 13. Core flux thermal spectrum calculated with the ENDF/B-VII.1 (left) and ENDF/B-VIII.0 reactor graphite 30% porous (right) cross section libraries using static conditions. Each tally bin’s uncertainty is less than 1%. The vertical lines aid in visualizing the softening of the neutron spectra due to the use of the ENDF/B-VIII.0 libraries.

Figure 14: Radial leakage spectrum from the core calculated with the reactor graphite and ENDF/B-VII.1 graphite libraries. Uncertainty in each energy bin tally is less than 1%.

In addition to the above, in the course of this project, methods for thermal neutron scattering analysis were developed that allow calculations of the scattering law to be performed on parallel computational clusters. Furthermore, such methods allow integration with codes like Serpent for on-the-fly analysis.
3) Major aspects in TREAT benchmark development

During this project, TREAT benchmarks based on the M2/M3 steady state and transient experiments were developed. The models related to these benchmarks have been completed. In addition, the basic benchmark (TREAT-FUND-RESR-003) was contributed to the International Reactor Physics Experiment Evaluation Project (IRPhEP) for inclusion in the International Handbook of Evaluated Reactor Physics Benchmark Experiments. As described, criticality calculations for the TREAT M2/M3CAL configuration were completed using the Serpent 2.1.29 Monte Carlo code. The benchmark models were implemented in the code. This model used the ENDF/B-VII.1 neutron cross section data for all materials except for the graphite thermal scattering law, where the ENDF/B-VIII.0 S(α,β) was used. In ENDF/B-VIII.0, graphite thermal scattering libraries are available for crystalline graphite, 10% porous reactor graphite, and 30% porous reactor graphite. Given the density of the TREAT graphite, the 30% porous reactor graphite library (tsl-reactor-graphite-30P.endf) was implemented.

Historically, calculated k\textsubscript{eff} values for graphite moderated systems have generally been lower than experimental values when using the ENDF/B-VII.1 libraries. Examples include the HTR-PROTEUS configurations and the associated benchmarks. The benchmark eigenvalues are consistently biased below the experimental values when calculated using the ENDF/B-VII.1 neutron cross sections. This benchmark also specifically cites the representation of the graphite as a possible contributor to the low eigenvalues. ENDF/B-VIII.0 addressed the graphite cross section by introducing new “reactor graphite” thermal scattering libraries. Reactor graphite exhibits a microstructure with a lower density than that of ideal graphite. In ENDF/B-VIII.0, the microstructural difference (and lower density) between reactor graphite and ideal graphite is represented as distributed porosity. Reactor graphite with a density less than 1.8 g/cm\textsuperscript{3} is represented using the 30% porous graphite library.

Comparing the ENDF/B-VII.1 and ENDF/B-VIII.0 total graphite cross sections in Fig. 12 above, significant improvement is seen in the ENDF/B-VIII.0 cross section when compared with experimental data. The introduction of the porosity increases the cross section, resulting in improved agreement with total cross section measurements below the Bragg cutoff (incoming neutron energy less than 0.002 eV). Implementing these cross sections in the HTR-PROTEUS benchmark, showed marked improvement in the comparison of the calculated and benchmark eigenvalues as seen in Fig. 15.

Fig. 15. HTR-PROTEUS benchmark core configurations evaluated using the ENDF/B-VII.1 carbon and ENDF/B-VIII.0 30% porous “reactor graphite” thermal scattering cross sections. The ENDF/B-VII.1 libraries were used for the remaining materials. The average deviation of the calculated k\textsubscript{eff} from the benchmark value is ±300pcm when the ENDF/B-VIII.0 30% porosity library is used. For ENDF/B-VII.1, the average deviation is -660 pcm.
Based on the above, the 30% porous reactor graphite library was used in the modeling of TREAT. This corresponds to the best representation of the nuclear reactor graphite used in both the reflector and fuel regions of the core.

Monte Carlo calculations in Serpent were completed using 100,000 particle histories per cycle, 1500 active cycles, and 100 skipped cycles for a total of 150,000,000 neutron histories in the $k_{\text{eff}}$ calculation. These run parameters resulted in converged source entropy. The calculated $k$-eigenvalue is given in Table 4. The calculated value for the TREAT reactor $k_{\text{eff}}$ value is greater than the experiment by 1.008% when using the 30% porous graphite cross sections, but it is still within the 1σ limit of the benchmark.

Table 4. Benchmark Eigenvalues. The analysis is performed using a hydrogen content of 510 ppm and boron content of 7.53 ppm in TREAT fuel.

<table>
<thead>
<tr>
<th>Neutron Cross Section Libraries</th>
<th>Calculated* $k_{\text{eff}} \pm \sigma$</th>
<th>Benchmark $k_{\text{eff}} \pm \sigma$</th>
<th>$(C-E)/E$ %</th>
<th>Difference (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF/B-VII.1 with ENDF/B-VIII.0 30% porous graphite</td>
<td>1.00900 ± 0.00007</td>
<td>0.99893 ± 0.01352</td>
<td>1.008</td>
<td>999</td>
</tr>
</tbody>
</table>

* Calculated $k_{\text{eff}}$ standard deviation from Monte Carlo statistical error.

Major sources of uncertainty in TREAT simulations include the large uncertainty in the hydrogen content and the boron concentration. Regardless of the graphite thermal scattering library, these quantities result in calculated $k_{\text{eff}}$ values that significantly deviate from the benchmark.

The hydrogen impurity in TREAT fuel is assumed to have an upper limit value of 970 ppm. Commonly, graphite materials begin with some hydrogen in the manufacturing process. This was true for TREAT where the initial hydrogen for the “green” blocks’ content was reported to be 1.5 wt%. After the graphitization process, typical graphite will have a hydrogen content of < 50 ppm. Using the two values of 50 ppm and 970 ppm to bound the range for the hydrogen impurity, an average of 510 ppm was used in the model. 1σ bounds were determined assuming a flat distribution between the maximum and minimum. Considering the impact of the hydrogen within the benchmark, the resulting $k_{\text{eff}}$ limits are given in Table 5 and compared with the experiment. It is anticipated that the hydrogen content of TREAT may be bound further after analyzing transient simulations in comparison to measurements.

Table 5. Benchmark Eigenvalues with Hydrogen Perturbation.

<table>
<thead>
<tr>
<th>Neutron Cross Section Libraries</th>
<th>Hydrogen Content</th>
<th>Calculated* $k_{\text{eff}} \pm \sigma$</th>
<th>Benchmark $k_{\text{eff}} \pm \sigma$</th>
<th>$(C-E)/E$ %</th>
<th>Difference (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF/B-VIII.0 30% porous graphite</td>
<td>244.4 ppm</td>
<td>1.00109 ± 0.00007</td>
<td>0.99893 ± 0.01352</td>
<td>0.22</td>
<td>+216</td>
</tr>
<tr>
<td>775.6 ppm</td>
<td>1.01501 ± 0.00007</td>
<td>0.99893 ± 0.01352</td>
<td>1.61</td>
<td>+1586</td>
<td></td>
</tr>
</tbody>
</table>

* Calculated $k_{\text{eff}}$ standard deviation from Monte Carlo statistical error.
Project Publications


