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RESEARCH IN SUPPORT OF TREAT KINETICS CALCULATIONS USING RATTLESNAKE/BISON COUPLING WITHIN MAMMOTH

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ABSTRACT

This paper summarizes key aspects of research in evaluation of modeling needs for TREAT transient simulation. Using measured data from transient experiments performed circa 1959 in a small, test core used for startup testing, MAMMOTH multi-physics simulations are performed to simulate the core transient behavior. MAMMOTH uses internal libraries from Rattlesnake to access the time-dependent transport solver and BISON libraries for fuel performance. These two applications inherent all of the MOOSE features, since they are built within the MOOSE multi-physics framework. Thus MAMMOTH can perform strongly coupled calculations to properly characterize the three-dimensional temperature-driven kinetics performance of the core during rapid power excursions. Early calculations were able to match the general shape of measured transient data but under-predicted peak power. Closer examination of the physics of the core and uncertainty associated with rod positioning led to calculations in which the best estimate of the actual measured reactor period was modeled. This correction resulted in outstanding agreement between measurements and coupled multi-physics simulation results.

Key Words: **TREAT, MAMMOTH, MOOSE, kinetics, multi-physics**

1. INTRODUCTION

The Transient Reactor Experiment And Test Facility (TREAT), located at Idaho National Laboratory (INL), is an air-cooled, thermal, graphite-moderated reactor designed to subject reactor fuels and structural materials to extreme transient power pulses simulating various types of power excursions and transient undercooling/loss of cooling accidents that could occur in a nuclear reactor. The reactor was operated from February 1959 until April 1994, generating over 720 MWh of energy for hundreds of unique experiments. [1,2] The TREAT core is build by appropriate arrangement of standard fuel elements, control elements, zircaloy-clad reflector elements, aluminum-clad reflector elements, and a number of other special-purpose elements, arranged on a 19x19 grid with a 10.16 cm (4 in) pitch. [3] Figure 1 provides a cutaway view of the TREAT core.

Transient testing of nuclear fuels is desired to improve predictive capability of accident scenarios by developing an experiment-based understanding of fuel, clad and moderator interaction, in support of various advanced fuel design initiatives. The U.S. Department of Energy Office of Nuclear Energy (DOE/NE) is preparing to resume operation of the Transient Reactor Test Facility. Based on ongoing efforts, it is expected that the facility will become operational by 2018, and resume transient testing before the end of the decade. [2]

TREAT testing involves placing cladded fuel pins or a small multi-pin assembly into the center of the core and subjecting them to short bursts of intense, high-power radiation. The fuel pins are typically loaded into an experiment test rig that, depending on the nature of the design, will contain different configurations of fuel targets and could contain coolant, pumps, heaters, pressurizers and various types of instrumentation. Fuel/clad failure, metal-water reactions, thermal interaction between overheated fuel and coolant, and the transient behavior of ceramic fuel for high temperature systems can be investigated. [4]

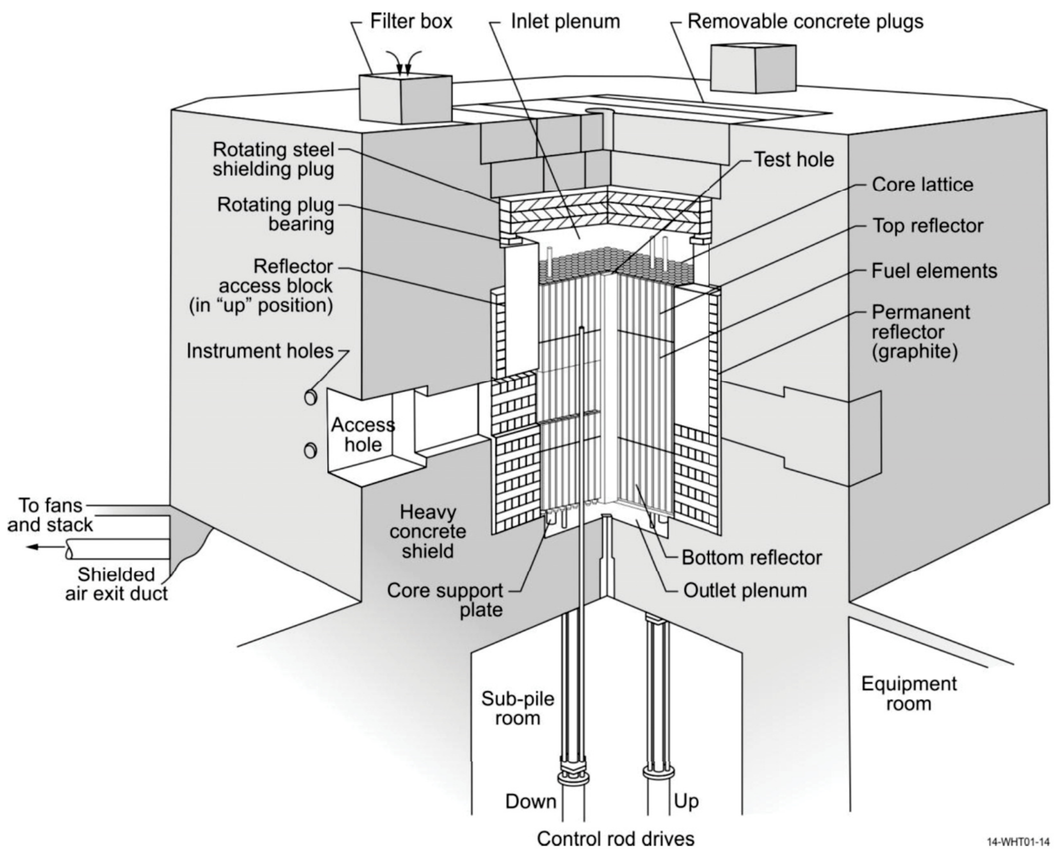


Figure 1. Cutaway Showing Internal Components within TREAT

Historical methods used for pre-transient calculations were very approximate and necessitated a number of reduced and full power tests to obtain correction factors to improve the prediction of the full power transient prior to the test itself. The use of modern modeling and simulation tools, capturing the multi-physics nature of TREAT operation and experimentation, has the potential for reducing the number of low and high power calibration tests needed prior to full power operations for a transient experiment. This would result in significant operational efficiency with corresponding cost savings, and would also lay the groundwork for improved fidelity in experiment design. Hence, INL is engaged in efforts to develop full multi-physics modeling capabilities to predict core transient behavior (power excursions with thermal feedback) and its coupling with experimental configurations, supported by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, within DOE/NE. [5,6]. This paper describes the state of multi-physics modeling for simulation of TREAT transient operations using a strongly coupled multi-physics method.

2. CORE MODELING APPROACH

TREAT provides a number of modeling challenges that are best addressed in a multi-physics simulation. Close coupling between neutron reaction rates and local temperature for a transient that lasts only a few seconds is critical to ensure that the time-dependent energy release is accurately predicted. The following subsections describe the general approach taken at INL to be able to accurately simulate TREAT transient behavior.

2.1 Multi-Physics Simulations

INL has developed high fidelity, strongly coupled multi-physics modeling under Multi-physics Object Oriented Simulation Environment (MOOSE) framework. [7] The MOOSE framework consists of several consistently designed, pluggable interfaces that may be used to simultaneously solve different physics phenomena. Internally, MOOSE utilizes the finite element method mathematical modeling technique due to its generality and wide applicability. In this work, the MOOSE-based transport solver Rattlesnake was used for neutron transport calculations with BISON for temperature calculations, both existentially residing as coupled objects within the MAMMOTH reactor physics tool, with user control over the nature of the coupling. [8-11]

A key feature of MOOSE-based applications is that a particular tool (in this case MAMMOTH) is compiled as a single executable code containing executable libraries for each component sub-application. In other words, within the MAMMOTH executable are embedded the full set of capabilities of BISON, Rattlesnake, and RELAP-7. [12] Communications between packages is performed in-core using shared memory managed by MOOSE algorithms. MAMMOTH also inherits the advances in each of the applications and enforces code compatibility for all applications. In the near future, additional sub-applications will be added to MAMMOTH to expand its range of capabilities. Although studies have been completed [13], this form of implicitly and explicitly coupled multi-physics capability existing in one code with a unified data/communications/solution structure is not known to exist for traditional reactor analysis applications. [14]

2.2 MAMMOTH Reactor Physics

In general MAMMOTH has great flexibility to solve complex reactor multi-physics problems. One approach is by implicitly solving a large system of interlinked nonlinear equations on the same mesh. This is known as the *strongly* coupled approach. These equations can be simultaneously solved with the Jacobian-Free Newton-Krylov (JFNK) method. [7] However, because of needs in some problems for solutions on different time scales, *strong* coupling is sometimes not optimal. Hence, a Picard iteration approach is available where each physics object within MAMMOTH solves its individual physics and has a coincident mesh with the other application(s). Data is shared between each object, coupling them using the MOOSE MultiApp system. [8,11] For this form of coupling, based on splitting the operator, additional outer iteration and time sub-steps can be applied to make the physics more consistent, and is referred to as a *tightly* coupled solution. Another type of operator splitting is known as the *loosely* or *weakly* coupled solution and is attained by setting the number of outer iterations to zero, thus the coupled solutions of the multi-physics fields are not converged at each time step

The MOOSE framework provides the necessary flexibility to perform multi-scale modeling where necessary, which will be imperative in experiment analysis and design. The general long-term technical objective of the currently MAMMOTH project in support of TREAT is to develop a set of high-resolution reactor physics and fuels performance models that can accurately predict the transient behavior of an in-core experiment as driven by a reactor transient. Current MAMMOTH development efforts are focused on capabilities that can be used in simulation of coupled neutron and thermal physics phenomena and scoping design and post-test experiment analysis for TREAT [5,6].

2.3 Problem Description

The primary goal in TREAT transient simulation to this date has been to demonstrate and ultimately validate MAMMOTH power transient simulations with coupled transport/heat transfer calculations using both Rattlesnake and BISON within MAMMOTH. Accurate representation of the shape and magnitude of the transient pulse will be essential to properly simulate the tightly coupled physics phenomena anticipated in experiment test rigs. The work included in this report describes recently completed calculations of a simple TREAT transient with thermal feedback. Efforts were made to capture all-important neutronic dimensions of a documented core configuration [15] with material-appropriate thermal properties, and to simulate the reactivity increase for a documented transient test; however, the work described herein does not necessarily rise to the level of benchmark quality. At present, the focus of this work is to begin to understand the dynamics of transient behavior with temperature feedback and to identify key modeling requirements needed to minimize error.

Following initial critical tests at startup, a series of transients were performed in 1960 on a “small core” to determine the operational characteristics of the reactor under transient conditions. Table XIII of Ref. 16 is provided in Fig. 2 and lists the reported parameters for a number of the temperature-limited transients. Based on the simplicity of the small core configuration, 159-element transient test 15 from this set was selected as a starting point; this test was a temperature limited transient experiment conducted with a total reactivity insertion of 1.55% Δk (\$2.16). Following the transient the reactor was returned to critical to determine the total reactivity change resulting from the transient. The design of a standard element is shown in Fig. 3; other elements have essentially the same form factor but have different material compositions. The full core, illustrated in Fig. 4, consisted of 159 fuel elements in a cylindrical configuration surrounded by Zircaloy-3 clad reflector elements for temperature protection. The additional Zircaloy-clad element show to the upper-right of the core contained the neutron source used for startup. The remaining elements were fully clad in aluminum. Although the reactivity change for the transient was provided, the initial control rod positioning data were not provided, so approximations were employed.

Transient	τ (sec)	Δk (%)	Peak Power (Mw)	Integrated Power (Mw-sec)	ΔT (°C)	Δk_T (%)	t (sec)	#
3	4.3	0.42	1.85	82	54.5		360	157
4	1.37	0.60	7.0	120	72		56	157
6	0.76	0.71	14	142	86	1.19	55	149
11	0.31	0.95	54	200	119	1.60	52	152
13	0.19	1.15	140	247	142	1.90	51	155
15	0.105	1.55	380	315	176	2.31	20	159
18	0.075	1.90	860	440	237	3.17	51	163

τ Period

Δk % reactivity added

ΔT Temperature rise of core center

Δk_T Total reactivity in transient

t Length of transient

\# Number of fuel elements in core

Figure 2. Summary of startup transient data. [16]

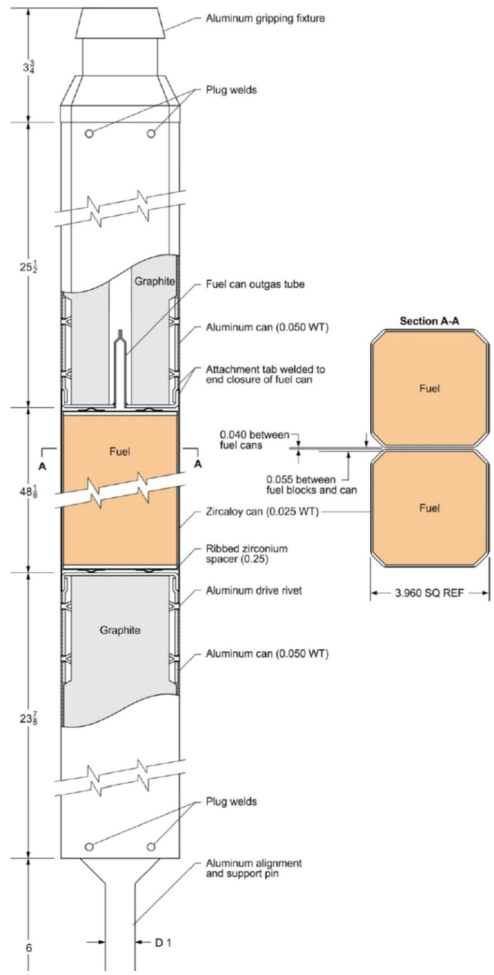


Figure 3. Standard TREAT fuel element. [17]

2.4 Modeling Approximations

The kinetics work described herein was preceded by an extensive study of modeling approximations including meshing, homogenization, cross-section generation methods and spatial effects on cross sections. [18]. A Serpent 2 [19] based reference calculation and a minimum critical core configuration were used to evaluate the various approximations [20]. For the current work the various radial regions of the assemblies were fully homogenized including the graphite fuel region, Zircaloy-3 clad, clad-fuel void region, and air channel outside the clad. The upper and lower reflector regions were similarly homogenized with the aluminum clad. TREAT control elements consist of a fuel element with a Zircaloy-3 lined cylindrical hole through the center through which passes a B_4C poisoned graphite rod with a graphite follower. The four locations that were rodded during the transient were simulated by homogenizing the boron through the control element (fuel and reflector regions); the amount of boron was varied to obtain a critical state and to obtain an eigenvalue of 1.0155 as the start and end points of the rod motion for the transient. The remaining four positions, for which the poisoned control rod was removed from the core prior to the transient, were modeled as homogenized fueled and unfueled graphite with appropriated volumes. In the figure, the set of

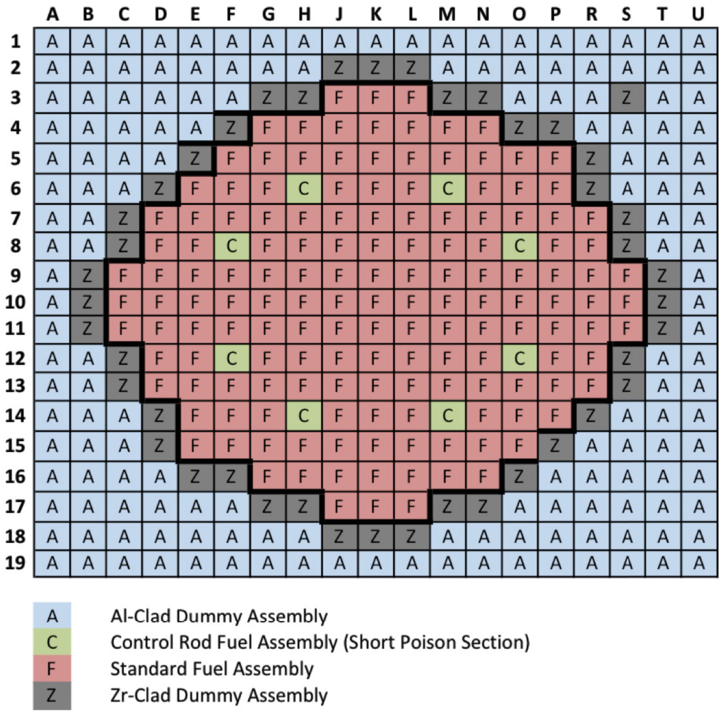
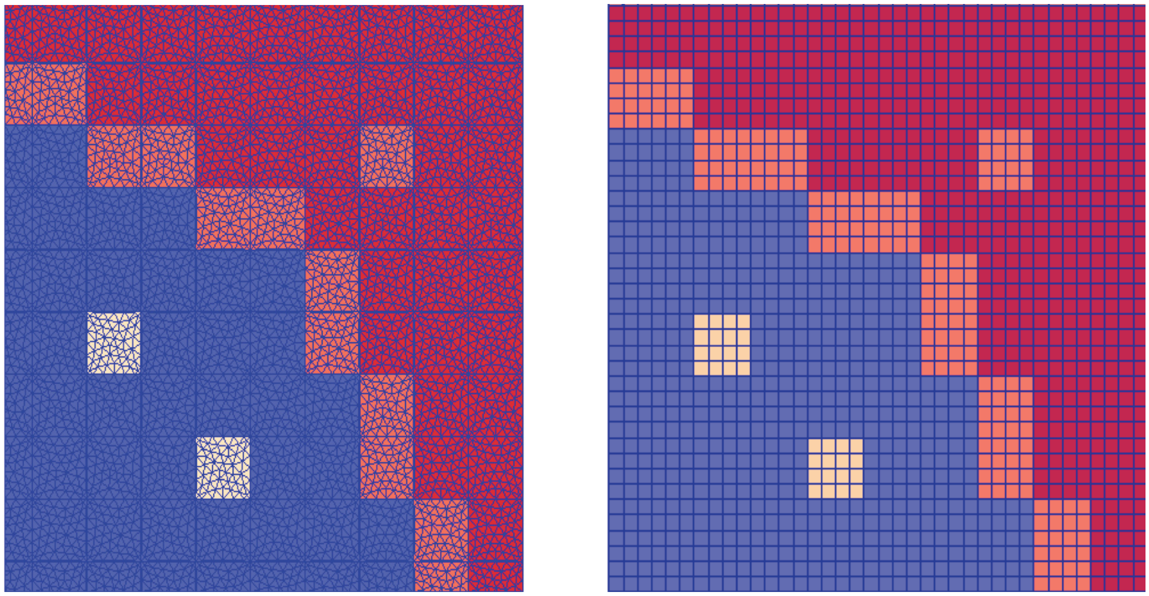


Figure 4. 159-element small core configuration of used for TREAT calibration transient #15.

rods in the upper right were used as the transient rods; the rods on the lower left across the core were set to take the core critical and were fixed during the transient. Rod at the upper left and lower right were fully withdrawn.

Serpent 2 was used to generate spectrally weighted multi-group cross sections. Because significant spectral changes are observed both radially and axially due to reflector and control rod effects, along with material changes axially, the core was divided into five cross section zones in the x-y plane and 7 zones axially. Macroscopic cross sections were generated as a function of temperature in 50K increments and tabulated; MAMMOTH is able to interpolate between these cross sections value to assign unique temperatures to each computational cell.

Since there is no significant deformation by the reactor fuel, such as in LWR fuel during operation, the thermal mesh may be assumed to be the same as the neutronic mesh for reactor simulations. This allows both loose or weak coupling and fully implicit or strong coupling to be applied for feedback calculations. A number of mesh approximations were employed in evaluating model performance. [18] Figure 5 (a) shows the mesh when air channels outside the clad were explicitly represented (to account for streaming effects); Figure 5 (b) shows sets of fully-homogenized elements, providing a simpler Cartesian mesh, both for the upper right quadrant of the core. Through use of diffusion coefficients correcting for axial streaming, the homogenized model was adjusted to match the explicit air channel model, which was then used for both Rattlesnake and BISON solvers. The temperature feedback for the full core was based on results from the adiabatic model and evaluated using two coupling approaches. Initially, thermal feedback was evaluated at the end of each time-step and not directly included in the residual evaluation, essentially using a loosely coupled



(a) (b)

Figure 5. Top down one-forth view of meshes for the 159-element core model. The left hand side (a) shows the mesh for explicit meshing of air channels; (b) shows the simpler mesh used with full homogenization.

operator splitting approach. The model was subsequently evaluated with a strongly coupled system, where temperatures were updated during the residual evaluation.

3. RESULTS

Initial simulations yielded encouraging results but significantly underestimated the core peak power. Subsequent sensitivity studies and analysis of measured data provided a better understanding of transient physics and allowed improvements in the ability to simulate measured behavior. The following subsection describes preliminary analyses reported in earlier studies [18]. This is followed by a summary of more recent analyses with significant improvement in core simulation results.

3.1 Initial Full Core Transient Calculations

The first set of results from the 159-element core transient calculations are shown in Figure 6 relative to reported power from the startup testing report. [16] A diffusion solution was performed using the Crank-Nicolson time integrator and with the time step set at 0.01 seconds. The peak power of 123.2 MW obtained in this simulation is significantly lower than that of the experiment, which is reported at 380 MW. The maximum temperature rise calculated for the core at 3 seconds was 140 K, and occurs at the core center. The temperature rise in location K-14 in the experiment was measured at 110 K [16]. Based on the radial distribution provided on the same report, the center assembly would be 30-40 degrees higher than location K-14, which is consistent with the model prediction. Figure 6 provides a qualitative comparison of the transient as computed by MAMMOTH and as provided in Fig. 30 of Ref 16. Although the peak powers are mismatched, the shape and timing of the computed transient are remarkably consistent with reported data. These results, published externally in Ref. 18, were subsequently revisited. An error in the value of the specific heat (C_p) for the fuel resulted in an under-prediction of the peak. However, when corrected, the peak power was found to be over-predicted. Next, it was realized that the homogenized mesh was providing too much graphite for the BISON model, and that the graphite fuel density specified for BISON needed to be reduced to account for this homogenization. This brought the peak power to within 30% of measured data (predicting high).

Realizing that it would be possible to continue to tweak parameters to obtain a better match to data, further manipulation was halted, and a new approach was proposed to step back and attempt to better understand the behavior of TREAT transients as a function of a more fundamental quantity: reactor period. This study is described in the following subsection.

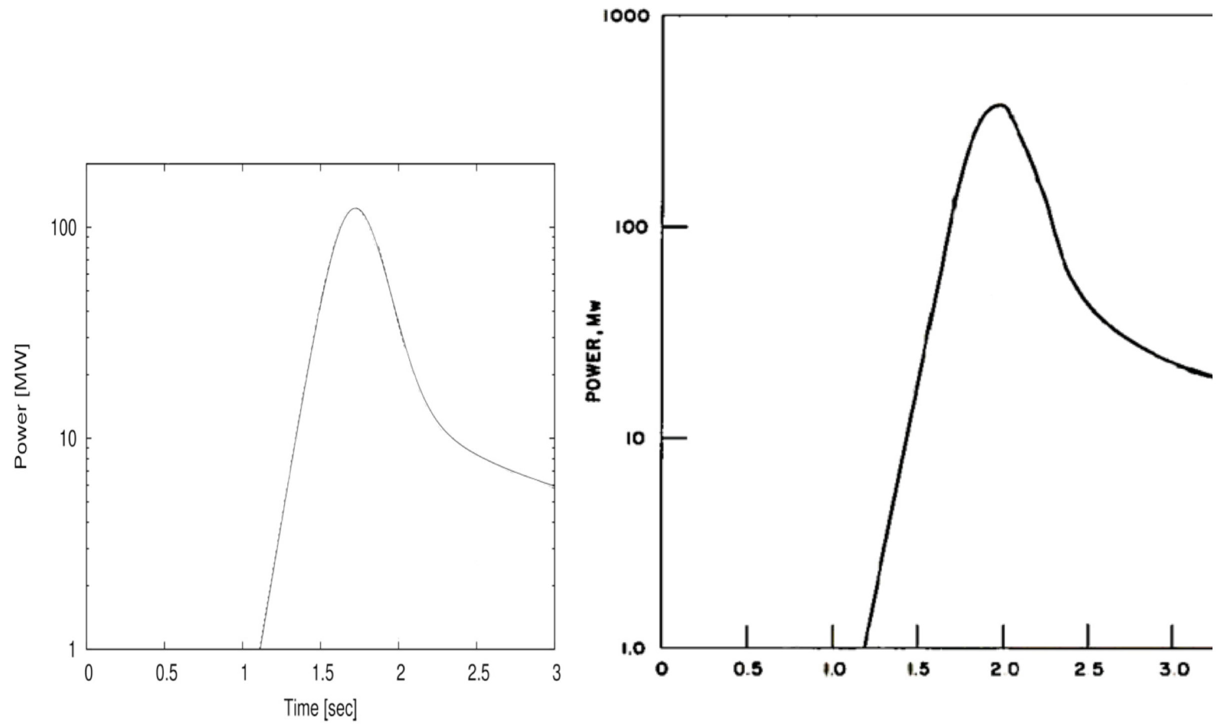


Figure 6. Core power for the 1.55% Δk transient, with a MAMMOTH diffusion solution with temperature feedback (left) and reported data [16] (right).

3.2 Further Study of Transient Simulation

The Test 15 transient was selected for the simplicity of the core. However, data from this 57-year old measurement were somewhat limited. Exact control rod positions were not known and control rods were approximated by varying boron concentrations to obtain k_{eff} values of 1.0 and 1.0155, yielding the reported reactivity change of 1.55%. However, while this is the value recorded, it is not clear how this value was derived. Measured data for detector currents were retrieved from an experiment logbook were analyzed to determine the period of the transient during the asymptotic power increase phase preceding temperature feedback effects. Figure 7 shows a log-linear plot of the power inferred (peak current used to normalize curves to a 380 MW response) from the currents reported from detectors identified as P-1 and P-2 in log data. It is clear that the two detectors measured different responses, but there is not enough information as to the reason for the differences. In addition, although the slope of the log power increase look the same, data fits indicate a very slight difference between the two. Table 1 lists the period measured by each detector, along with the associated reactivity computed using the in-hour equation and the reported reactor parameters reported for steady state. The P-2 detector data indicates a reactivity increase of 0.01552, which is consistent with reported reactivity, while data from P-1 indicates a 0.01481. The values do not seem significantly different, but because power is growing exponentially the small difference in reactivity that results from the period can result in a large power difference. For example, assume that the time between 0.75 and 1.25 s represents an asymptotic period without feedback (the core average temperature begins to increase around 1.3 s in this simulation). The relative power increase $P/P_0 = e^{(t/T)}$, where T is the period and t is the time elapsed, the 0.103 s period derived from P-1 would result in a power increase by a factor of 87 over this period; the 0.112 s period would result in an increase by a factor of 128, 48% higher. Thus small change in reactivity, resulting from slightly different periods, will result in a significant change in power. Hence, the under-prediction of the peak power described in Sect. 3.1 could easily result from a small misestimating of the true reactivity change, due to measurement uncertainties, influenced in part due to lack of precise data on rod positioning.

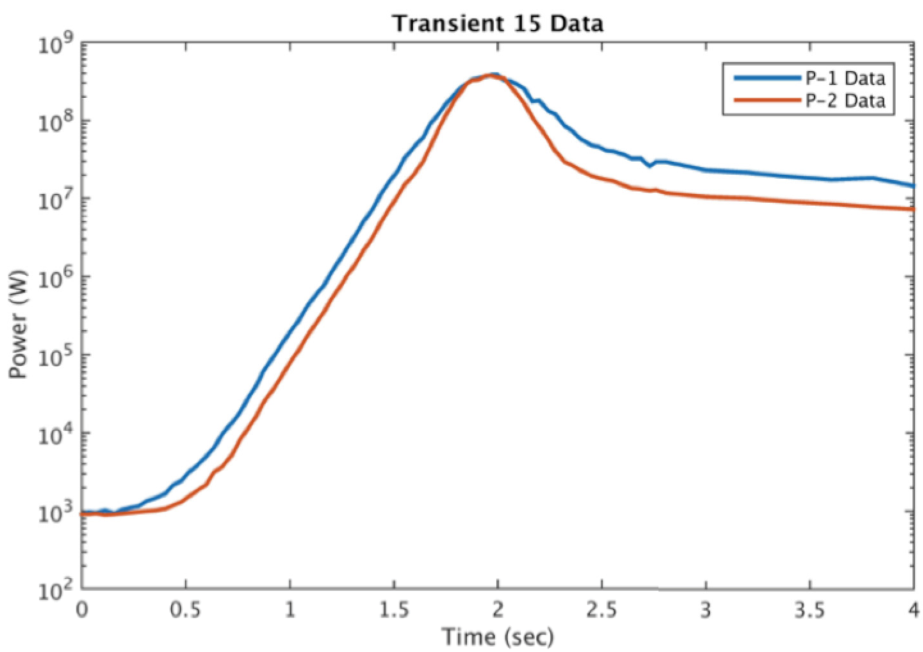


Figure 7. Detector current from P-1 and P-2 detectors from Transient 15, scaled to an initial power of 910 W.

Table 1. Period and Corresponding Reactivity

Period	Reactivity
P-1: 0.112 sec (maximum) +/- 4%	0.01481
P-2: 0.103 sec (minimum) +/- 1.5%	0.01552
Average: 0.1075 sec	0.01515

Because reactivity is calculated from the measured period along with kinetics parameters measured in the pre-transient core, and the lack of data to simulate the actual rod positions and motions in the measured transient, it is more meaningful to study a core simulation based on the power period. However, with two detectors providing different periods, it is not clear which is the more appropriate period. It is not unreasonable to assume that best estimate of the period is the average of the two measured periods. Indeed, the approach used to determine the period from the reported current data has its own uncertainty, so the reported periods themselves have an associated uncertainty based on the estimated time range for asymptotic period and the goodness of fit for the data; estimated uncertainties are provided in Table 1 for each period. Note that the P-2 response gives a period close to 1.55%; however, this number was derived (using the reactivity or "inhour" equation [21]) assuming values for the neutron lifetime and delayed neutron parameters from TREAT literature [22]. It is not known what values (primarily the neutron lifetime) were used in the original calculations, so this may correspond to a slightly different period. Further, there is an approximately 20 pcm difference for the 1.55% transient, depending on the type of inhour formulation that is used. The difference is the interpretation of neutron lifetime vs generation time. The lifetime estimate is perhaps better suited for this application.

To better understand the relationship between peak power and the asymptotic period of the transient, the earlier simulation was modified by creating three new cases, in which the initiating reactivity increase was varied for each case to match the periods of Table 1. Once the needed reactivity change was determined, the transient was rerun using BISON-calculated temperatures for thermal feedback. Figure 8 illustrates the results of the simulated power transients relative to the powers inferred from P-1 and P-2 detectors. Overall, the three simulations are in good agreement with the P-1 results. P-2 results are in generally good agreement up to the power peak, but show a significantly lower power than predicted by MAMMOTH after the power has peaked. Figure 9 shows the results from the average period simulation versus P-1 data, showing excellent agreement. The reasons for this behavior on the P-2 measurement is not clear, nor can it be determined which detector best captures the actual transient behavior. Agreement with P-1 results is encouraging, but does not ensure that the actual transient behavior has been reproduced. However, the fact that the thermal feedback model closely follows the behavior of both detector responses up to the power peak (and P-1 after this point) indicates that the coupled multi-physics aspect of the simulation is giving a representative response.

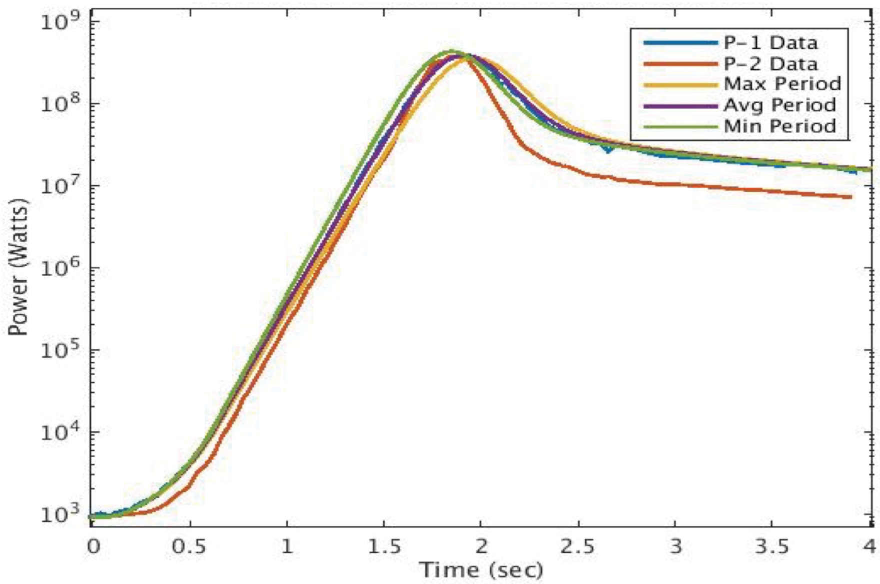


Figure 8. MAMMOTH calculations for which simulation periods were matched to period data obtained from Transient 15 measurements. Max, Min and Avg periods correspond to the maximum, minimum and average periods provided in Table 1.

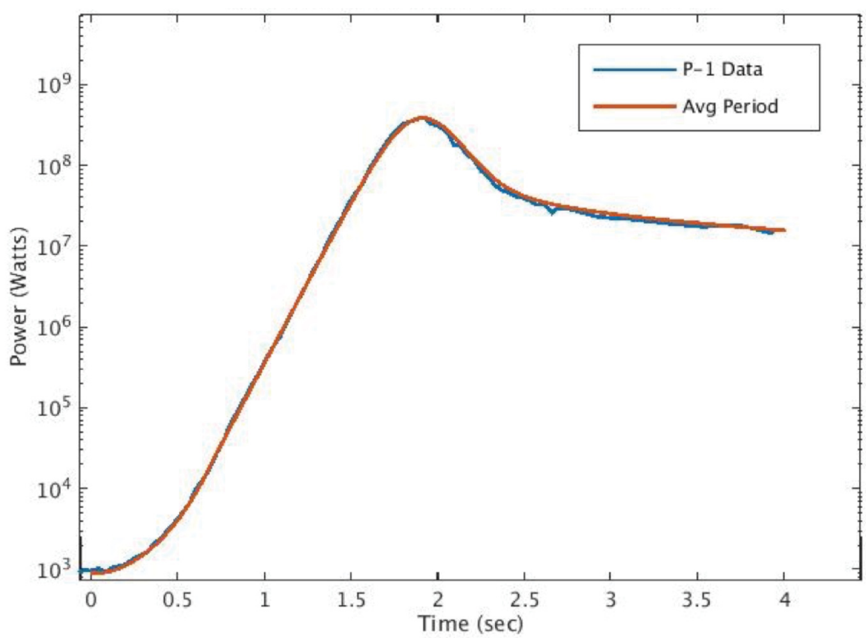


Figure 9. MAMMOTH calculations using the average period vs P-1 detector data.

Note that the power trace plots are logarithmic on the y-axis because of the scale of the power change over the transient. This also tends to hide differences at the power peak. Table 2 provides the peak power predicted in each simulation. It also provides integral powers and maximum temperature change for the core center. Reported results from Test 15 are also provided. Uncertainties in measured data were not provided. However, we still observe the best agreement for the calculation based on the average period. The close agreement on power, approximately 1% high for the average period case, is largely fortuitous – power predictions were historically assumed to be plus or minus 10%. Because the peak power is strongly coupled to the temperature increase, we also see agreement on the predicted temperature increase for the same case. However, there is a significant shortfall in the integral. Over the longer term (4 - 10s, not shown in the figure), the three simulations predict a lower power than the measured data. On a log plot this difference is not obvious and hence not shown here.

Table 2. Power and Temperature Results from Test 15 Measurements and from Three MAMMOTH Simulations.

Period (sec)	Peak Power (MW)	Peak Power % Diff	Integral Power (MJ)	Integral Power (% Diff)	ΔT max (K)	ΔT max (% Diff)
Test 15[16]	**380**	**-**	**315**	**-**	**176**	**-**
0.1033 (Min)	425	11.7	291	7.6	180	2.2
0.1082 (Avg)	384	1.1	281	10.7	174	1.3
0.1126 (Max)	355	6.5	268	14.9	166	5.8

4. CONCLUSIONS

The preliminary work completed to date has provided considerable insight into the behavior of TREAT and the modeling requirements to be able to simulate the reactor under transient conditions. The work described in [18, 20] laid the groundwork for the present effort. Early research focused on development of appropriate modeling parameters and processing requirements to accurately calculate the solution first for an infinite lattice of assemblies then for a known critical core configuration, relative to reference Serpent calculations for the same configurations. That work also demonstrated the coupling of BISON and Rattlesnake within MAMMOTH for infinite lattice models. In the current work, the MAMMOTH multi-physics solver was applied to a simulation of an early test transient configuration. First efforts to simulate the core and compare to measured data were encouraging in demonstrating the appropriate behavior with coupled thermal feedback and a transient shape similar to experimental data, but topped out too soon and under-predicted the peak power for the transient. After closer inspection, it was determined that small differences in reactivity measurement can result from different relative positioning of rods; this small difference could result in a significantly different power peak. It was then demonstrated that a marked improvement is seen in power predictions when the period of the excursion (the only truly measured data) is matched, transient simulations are in much closer agreement to measurement data. In this work, the agreement between prediction and measured data is perhaps more coincidental than real, given the expected uncertainty in detector responses and the actual power peak.

Much work remains to be done in modeling and simulation development within MOOSE. A model is being developed for the current TREAT core configuration, in which the most recent measurements were performed in the M8 calibration series in the early 1990s [23]. The simulation efforts will focus on not only transient data but also measured test wires and fuel rods used in the calibration work within the central experiment vessel. Rod data are also available for these measurements. The challenge here will be that the core is much more complex – three sets of control rods are present, the active core is significantly larger, and a unfueled, air-filled central slot exists between the target vessel and a hodoscope located outside the reactor. Streaming effects in this slot will challenge existing calculational methods, and advanced methods will be needed to account for streaming effects. In addition, work is ongoing to develop an improved quasi-static (IQS) solver for Rattlesnake to allow calculations to be performed with larger time steps without significant loss of accuracy. Finally, parallel efforts are underway to test and validate MAMMOTH calculations in which RELAP-7 is also included in the multi-physics solution. Fully coupled RELAP-7, BISON and Rattlesnake solvers will be necessary to accurately simulate flow loop experiments that are planned for future flow tests.

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