INL/CON-15-35771
PREPRINT

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ANS Winter Meeting

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November 2015

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U.S. Department of Energy
National Laboratory
operated by
Battelle Energy Alliance

Multi-Physics Simulation of TREAT Kinetics using MAMMOTH

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I. Introduction

With the advent of next generation reactor systems and new fuel designs, the U.S. Department of Energy (DOE) has identified the need for the resumption of transient testing of nuclear fuels. DOE has decided that the Transient Reactor Test Facility (TREAT) at Idaho National Laboratory (INL) is best suited for future testing. TREAT is a thermal neutron spectrum nuclear test facility that is designed to test nuclear fuels in transient scenarios. These specific fuels transient tests range from simple temperature transients to full fuel melt accidents.

The current TREAT core is driven by highly enriched uranium (HEU) dispersed in a graphite matrix (1:10000 ^{235}U/C atom ratio). At the center of the core, fuel is removed allowing for the insertion of an experimental test vehicle. TREAT's design provides experimental flexibility and inherent safety during neutron pulsing. This safety stems from the graphite in the driver fuel having a strong negative temperature coefficient of reactivity resulting from a thermal Maxwellian shift with increased leakage, as well as graphite acting as a temperature sink. Air cooling is available, but is generally used post-transient for heat removal.

DOE and INL have expressed a desire to develop a simulation capability that will accurately model the experiments before they are irradiated at the facility, with an emphasis on effective and safe operation while minimizing experimental time and cost. At INL, the Multi-physics Object Oriented Simulation Environment (MOOSE) [1] has been selected as the model development framework for this work.

This paper describes the results of preliminary simulations of a TREAT fuel element under transient conditions using the MOOSE-based MAMMOTH reactor physics tool.

II. Modeling with MAMMOTH

The MOOSE based reactor physics tool MAMMOTH provides the capability to seamlessly couple the neutron transport application RATTLESNAKE to the fuels performance application BISON to produce a higher fidelity tool for core simulations. RATTLESNAKE solves the time dependent form of the self-adjoint angular flux transport equation (SAAF), derived from the linearized Boltzmann transport equation. BISON solves the coupled thermo-mechanical equations for a fuel-clad system. The coupling within the MOOSE framework allows both applications to solve their respective systems on aligned and unaligned unstructured finite element meshes. MAMMOTH provides BISON with the power density calculated by RATTLESNAKE; the temperature distribution from BISON is used by MAMMOTH to update cross sections for RATTLESNAKE.

Both implicit coupling and explicit (Picard iteration) solution methods are available with the MOOSE framework. For implicit coupling, all equations are solved simultaneously by MOOSE solvers and are thus time consistent in terms of coupling. In the explicit mode, MAMMOTH transfers data to BISON with the MOOSE MultiApp transfer system; BISON in turn returns data in the same manner. The number of Picard iterations selected determines the degree of coupling between solutions. A single Picard iteration would be equivalent to an operator split solution or inconsistent loose coupling in terms of accuracy. Increasing the number of iterations to a fully converged solution is termed strong coupling and if correctly coupled will converge to the same solution as the implicit mode. [3]

MOOSE also provides support for parallel, distributed computing. The calculations were

performed on the INL Falcon high performance computing cluster, a 16,416-core SGI ICE X distributed memory system, using varying numbers of nodes and cores depending on problem size.

A small team of personnel from Oregon State University (OSU) is collaborating with INL in developing TREAT element models for transient simulations. A companion paper describes a study of meshing and solution approaches for steady state eigenvalue calculations. In this work, we examine the performance of three-dimensional MAMMOTH transient calculations for a single TREAT fuel element in an infinite lattice configuration. The fuel element model explicitly represents a 121.92 cm (4') fuel region; a cross section of the fuel region is show in Fig. 1. Above and below the core are located Zircaloy-3 spacer region that thermally separate the fuel region from ~60.96 cm (2') graphite reflectors. The fuel region is clad in Zircaloy-3 while the reflector is clad with aluminum. The entire element is centered within a 10.16 cm (4") square of air, ~250 cm tall. Reflective boundary conditions were applied on all four sides of the element, with vacuum above and below the reflector regions.

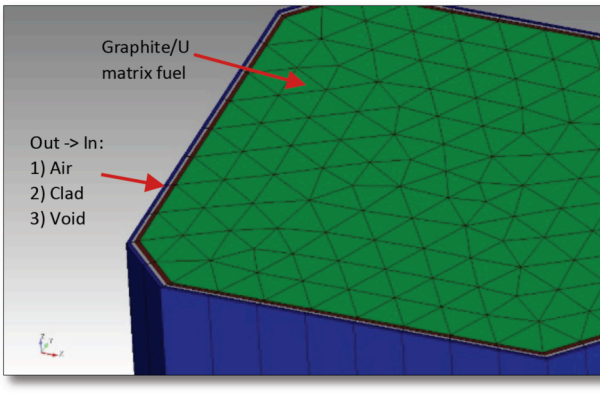

Fig. 1: Meshed cross section of TREAT element fuel region.

III. Methodology

RATTLESNAKE solves the time dependent version of the transport equation with prompt and delayed neutrons. Six-group delayed neutron data were generated for TREAT fuel with DRAGON5 [2]. In this work temporal differencing was performed using an implicit Euler method available within MOOSE. Quasi-static approaches were not employed; an implicit transport solution as performed at each time step in a simulated transient.

In the calculations reported here, the ^{10}B concentration was set at 9.99×10^{-7} atoms/b-cm to obtain an initial critical condition. In all transients, the ^{10}B concentration was linearly decreased to a value of 9.65×10^{-7} atoms/b-cm between 0.01 and 0.015 s after the beginning of the simulation. For all transients the initial temperature was assumed to be 303K; for coupled calculation with feedback fuel temperatures varied with time and space within the fuel element, with adiabatic conditions assumed as boundary conditions for the thermal solution. A steady state flux corresponding to a 10 kW initial power was assumed

Although MOOSE supports varying time step sizes specified in input or with an adaptive adjustment, the calculations performed here used a fixed 0.005 s time step, unless otherwise specified. Only the first 2.0 s of this simulation were calculated.

Cross sections were prepared for each material as a function of temperature and with varying boron content in the fuel, using the process described in [2], with SPH corrections. In this model, control rod motion is simulated by varying the boron content within the fuel.

IV. Analyses

The first set of calculations was performed using RATTLESNAKE only, i.e., with no thermal feedback from BISON. This calculation was performed simply to test the functionality of kinetics calculations within RATTLESNAKE with externally generated cross sections and kinetics parameters and to provide a point of comparison for calculations with thermal feedback. For these calculations, the "reactor" consisted of an infinite lattice of the finite-height and axially reflected fuel elements described earlier. As mentioned earlier, the transient was initiated with boron removal over a short period. To simulate the behavior of thermal feedback, the boron was slowly reintroduced into the model from 0.015 s to 1.0 s then the core allowed to return to equilibrium.

The second set of analyses performed true multi-physics calculations in which various coupling

modes within MAMMOTH were compared, using RATTLESNAKE and BISON objects. A fully implicit calculation was performed and compared to solutions with 1, 2, and 4 Picard iterations.

Finally, the implicit Euler time differencing approximation was evaluated with decreasing time step sizes. Although a more accurate Crank-Nicolson method is available in MOOSE, this method is not currently compatible with delayed neutron contributions. Initial calculations were performed using 0.005 s time steps, decreasing by a factor of 0.5, i.e., 0.005, 0.0025, 0.00125, down to 0.00015625 s.

V. Results

V.a Verification of Transient without Feedback

Figure 2 shows the results of a standalone RATTLESNAKE calculation with content (^{10}B) driven reactivity changes. The plot shows the ^{10}B concentration (red) and the power transient from an

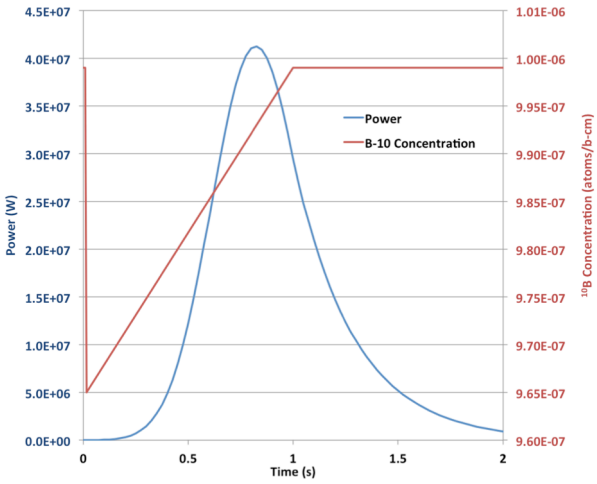

Fig. 2: MAMMOTH (RATTLESNAKE) simulation of simple time-dependent reactivity changes

initial critical steady-state power level of 10^4 W (blue). As the transient is initiated the power begins to increase exponentially, but the exponential rise is tempered with time as boron is reintroduced. Eventually the power peaks when a prompt critical state is reached, and decreases to a new equilibrium power as delayed critical is slowly re-established.

V.b Thermal/Neutronic Coupling

Although MAMMOTH provides the ability to perform implicit coupling, there are times where implicit coupling is not appropriate or possible. Additionally, it is important to understand the importance of converging thermal and neutron solutions in TREAT transient calculations.

In this set of calculations, MAMMOTH was exercised in both implicit and explicit coupling modes with coupling between BISON and RATTLESNAKE. The same initial transient used in Sect. V.a is simulated with boron removal. However, in this case, thermal feedback is provided using BISON. Cross sections are updated at each time step based on temperature increases, resulting in negative feedback. The results are shown in Fig. 3 for each of five different simulations. The fully implicit transient solution is shown by the dashed line. Solid colored lines illustrate the transient calculated using prescribed numbers of coupled

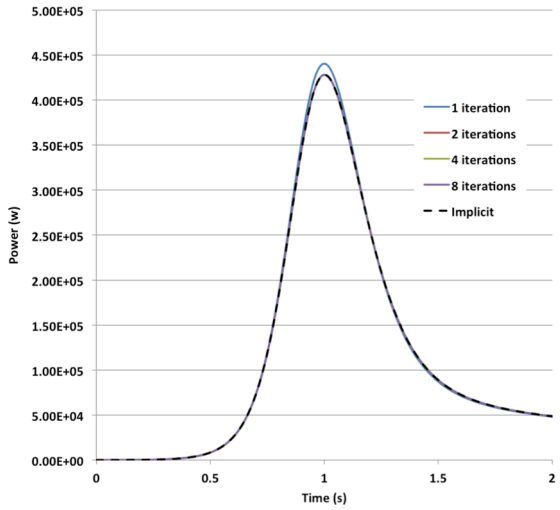

Fig. 3: Coupling approximations within MAMMOTH (RATTLESNAKE/BISON) relative to implicit coupling for a simulated TREAT transient.

iterations. One iteration (operator split) overestimates the power peak by ~3%, two iterations by less than 0.1%, and additional iterations all less than 0.005%. The explicitly coupled solution was effectively converged with four Picard iterations.

Note that the shape of the initial transient is the same as that shown the earlier analysis plotted in

Fig. 2, although the magnitude and timing of the peak are different because of the different feedback mechanism.

V.c Convergence with Time Step Size

The final study described here was to assess the impact of time step size on the transient calculation in coupled RATTLESNAKE-BISON simulations. Because MAMMOTH currently uses the lower order implicit Euler time differencing approach, its accuracy is limited by time step size. As would be expected, solutions converge to a single solution as time step sizes get smaller. As illustrated in Fig. 4, time step sizes of 0.005 s and 0.0025 s under-predict the magnitude of the transient peak (less than 0.5% error) and show the peak time occurring slightly earlier in the transient. Figure 5 provides a close-up view of the peak of the transient to highly these differences. Mathematically it is clear that a very small time step is desirable. Nevertheless, the error associated with larger time steps would likely be dwarfed by other modeling approximations in a TREAT model.

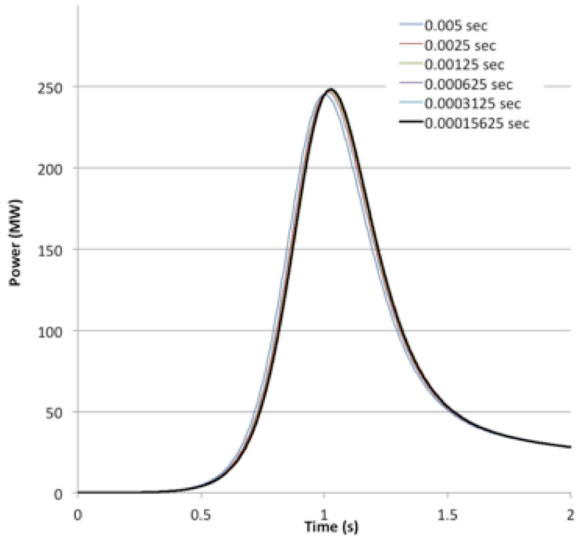

Fig. 4: Effect of time step size within MAMMOTH (RATTLESNAKE/BISON) relative to implicit coupling for a simulated TREAT transient.

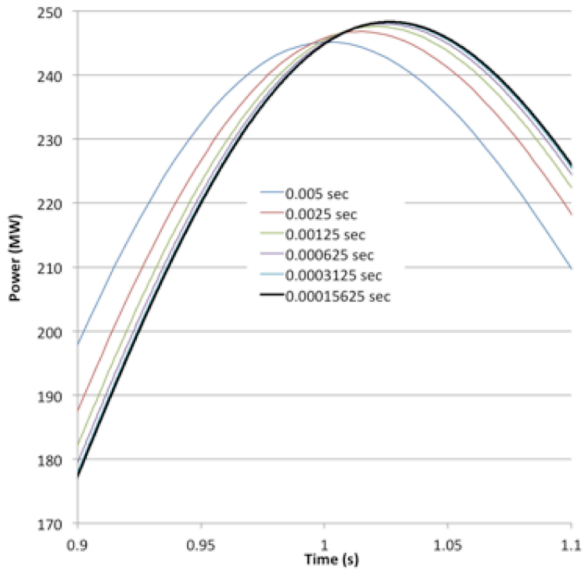

Fig. 5: Close-up view of transient peaks from MAMMOTH simulation.

VI. Future Work

The results presented here represent very preliminary findings for studies of feedback effects and transport/thermal coupling within MAMMOTH. No claims are made as to the accuracy of the transient simulation, as the prescribed transient represents an academic exercise. Future work will involve full core modeling to validate calculations against historical measurements. Code-to-code comparisons are also planned using TDKENO [4] and infinite medium analytical solutions.

The calculation performed here used the diffusion solution mode within RATTLESNAKE. Work is ongoing to evaluate cross sections, comparing diffusion, spherical harmonics and discrete ordinates solution modes. The effect of spatially varying cross sections due to reflector effects is also being evaluated. Finally, development work has been initiated to support an improve quasi-static (IQS) solver for MAMMOTH, as an option to improve the time-dependent performance of MAMMOTH.

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