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A.X. Zabriskie and W. Marcum
(Oregon State University)

B. Baker, J. Ortensi, M.D. DeHart
(Idaho National Laboratory)

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SELF-LIMITING TRANSIENT PULSE SIMULATION METHOD EXHIBITING TIME LAG PHENOMENON USING MAMMOTH

Adam X. Zabriskie¹, Benjamin Baker², Javier Ortensi², Mark D. DeHart², and Wade Marcum¹

¹Oregon State University
1500 SW Jefferson St.
Corvallis, OR 97331

²Idaho National Laboratory
2525 Fremont Ave
Idaho Falls, ID 83402

zabrisad@onid.oregonstate.edu, benjamin.baker@inl.gov, javier.ortensi@inl.gov,
mark.dehart@inl.gov, Wade.Marcum@oregonstate.edu

ABSTRACT

Coupling of multi-physics and multi-scale allows the exploration of phenomenon not previously studied with high fidelity. The heat diffusion time lag in TREAT-like fuel requires both multi-physics and multi-scale coupling to model the full transient behavior. The reactor physics code MAMMOTH, which has the ability to couple the heat conduction equation and the neutron diffusion equation, simulated a self-limiting transient pulse meeting these requirements. The MOOSE MultiApp system allowed the coupling of many micro-scale simulations with a single macro-scale simulation. The micro-scale geometry was a 0.0044 cm diameter UO₂ fuel grain surrounded by a graphite moderator. The macro-scale geometry was a homogeneous fuel with the same isotope ratio of the micro-scale material surrounded by a graphite reflector. Two temperature-dependent two energy group cross-section libraries were computed using Serpent 2 for use in MAMMOTH. Both the homogeneous unit cell and heterogeneous unit cell cross-section library had infinite reactor boundary conditions. The macro-scale simulation had finite boundary conditions. By varying the feedback temperature, macro or micro, given to the cross-sections, the effect of the time lag was explored using a Picard coupling method. The time lag increases the peak power density by 9 % to 10 % and the energy deposited by 8 % to 9 %. The effect of differing grain and moderator temperature at the micro-scale was also explored showing differences in time lag behavior. Future research will improve the fidelity of the method through representative macro-scale geometries, temperature-dependent cross-sections, and greater energy group resolution.

KEYWORDS: Transient, MAMMOTH, Multi-physics, Time lag

1. INTRODUCTION

The value of any simulation may be measured by the fidelity of that simulation to the actual world. To describe and predict the physical world, governing equations and models of physics have been developed.

The comparison of predictions to experimental measurements helps improve the physics models. The predictions from these models then highlight areas needing more experimentation or supporting data. In an effort to increase fidelity, multi-physics simulations, which couple governing equations together, have been developed; MAMMOTH is such a code, coupling many of the physics directly related to nuclear reactor simulation [1].

MAMMOTH is built upon the Multi-physics Object Oriented Simulation Environment (MOOSE) framework [2]. The MOOSE framework provides coupling of equations at different domain scales through the MultiApp system [1], which enables the seamless transfer of variables and other information between distinct simulations. MAMMOTH can couple the diffusion equation approximation of the neutron transport equation [3] and the solid body energy (heat) equation [1].

Phenomenon due to multi-physics coupling may be explored with MAMMOTH simulations. Consider a reactor fuel containing small particles or grains of fuel material dispersed in a matrix of moderator material. In the current work, the time required for heat to diffuse from a fuel grain into the surrounding moderator in nuclear fuel is of interest; heat is generated by fission in the fuel grain, but the temperature feedback is from the surrounding moderator. This time lag affects the neutron spectrum due to the delay of thermal feedback effects. Because of this, modeling of energy deposition rates as a result of fission-produced heat is a complex coupled phenomenon of particular interest during a power pulse in such a fuel structure.

The complexity becomes most evident when comparing the amount of variation of the two coupled governing equations with respect to length scale. The mean free path of neutrons in graphite is on the order of centimeters, thus a proper discretization to obtain the solution for the neutron diffusion equation must have elements small enough to resolve centimeter changes in neutron flux. Contrast that requirement to the length scales associated with the heat equation; the size of the fuel grains in the moderator are on the order of micrometers. To resolve the temperature solution, elements need to be smaller than the size of the fuel grains. A method to handle the multi-physics and multi-scale requirements for obtaining a solution for both the neutron flux and temperature field was developed using the MOOSE MultiApp system to link together simulations at different scales.

The MultiApp system relies on the transfer of information between apps to achieve multi-physics and multi-scale coupling. Apps are simulations, which require information available through transfers from other apps. Multiple micro-scale apps to resolve the temperature solution were positioned throughout a single macro-scale app resolving the neutron flux solution. The micro-scale apps formed a grid within the macro-scale fuel block. When transferring the power density from fission to the micro-scale app, the macro-scale app was sampled at each location giving a unique power density based on the neutron flux at that location. The feedback temperature was passed from the micro-scale app to the macro-scale app providing a field of values on the macro-scale fuel block of feedback temperatures. Feedback temperature values needed at locations without a micro-scale value were interpolated from the rest of the field. More micro-scale positions would increase fidelity with a finer grid and less interpolation. Picard iterations converged all apps on each time step before advancing to the next time step.

2. TIME LAG PHENOMENON DESCRIPTION

To explore the time lag phenomenon through MAMMOTH simulations, a scenario is explored in which the reactor fuel is composed of uranium dioxide (UO_2) grains suspended in a graphite moderator matrix. This type of fuel configuration powers the Transient Reactor Test (TREAT) facility at Idaho National Laboratory (INL), which has the ability to conduct temperature controlled pulse transients subjecting experiments to transient conditions [4].

To ensure safe reactor operation following any kind of power increase in a nuclear reactor, a negative feedback is required. Currently, with the use of highly enriched uranium (HEU) fuel, TREAT achieves this feedback requirement with a shift in the thermal Maxwellian distribution of the neutron spectrum to higher energies as the graphite moderator increases in temperature. The neutrons in thermal quasi-equilibrium with the reactor naturally increase in energy with the hotter (more energetic) graphite moderator. This shift in the spectrum to higher energies is often called “spectral hardening.” Because TREAT fuel has a carbon to uranium (C:U) ratio of about 10,000:1, the temperature of the graphite governs the neutron spectrum shift.

Figure 1 shows three important cross-sections for neutrons in TREAT-like fuel. With a hardened spectrum (increased average energy in the thermal range), a decrease in fissions for ^{235}U decreases the production of new neutrons and increases the probability that neutrons will either leak out of the reactor or be absorbed by either ^{238}U or other structural materials (such as graphite). The current TREAT HEU fuel is enriched to 93.1 wt% ^{235}U [4] and hence has a low ^{238}U content. This makes ^{238}U inconsequential and non-fuel materials are the predominant source of parasitic absorption.

If large enough, the fuel grains within the graphite matrix may capture a large portion of the fission energy deposited by fission fragments. The deposition location differs with fuel grains explicitly modeled (heterogeneous) versus simulation with the fuel grains homogenized with the graphite moderator. This homogenous material includes all atomic densities of all the isotopes lumped together in the fuel meat. The homogeneous simulation assumes that fission energy is deposited directly into the graphite, providing virtually instantaneous thermal feedback for the transient. With the low thermal conductivity of UO_2 , the more physically representative heterogeneous simulation delays the time at which the graphite temperature responds, affecting the time-dependent response of the transient. Using only the heat conduction equation with spherical fuel particles of varying diameter in graphite, a time lag delay resulting from heat diffusion from the fuel particle to the surrounding graphite has been demonstrated without feedback analytically [5] and with simulations [6].

Other efforts have accounted for the fission fragment damage effect on the thermal conductivity of the bulk fuel mixture [7] and the damage effect on increasing transients exhibiting time lag [8]. A common assumption, also assumed in this work, is that the heat energy from fission is entirely deposited in the fuel grain. Previous time lag work has mainly dealt with the no feedback transient or has provided the pulse power shape without coupling. With multi-physics coupling, this work shows the time lag effect throughout the transient pulse. This work assumes no radiation damage degradation or temperature-dependence of material properties.

To increase fidelity and include temperature feedback for this phenomenon, the heterogeneous and homogeneous simulations were compared for a spherical fuel grain using a multi-physics, multi-scale approach. Due to the computational limits, the problem domain was divided into a homogeneous macro-scale core size domain and a heterogeneous micro-scale fuel grain unit cell size, each being an “app” in the MOOSE MultiApp system.

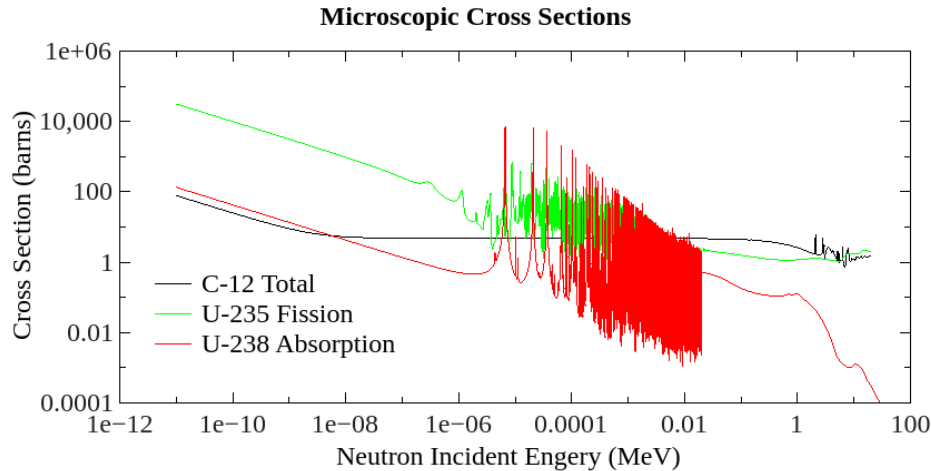


Figure 1. Microscopic cross-sections for three isotopes found in TREAT fuel.

3. MODEL DESCRIPTION

The problem domain was divided by physical size to allow for heterogeneity at smaller scales, with finite reactor effects, such as neutron leakage, at larger scales. The micro-scale unit cell (micro-app) is used to form cross-section libraries and provide a heat diffusion solution. The macro-scale reflected fuel block (macro-app) provides the neutron diffusion solution, which includes the power density from fission and bulk heat transfer to the reflector.

3.1. Micro-App Domain

The explicit modeling of individual spherical fuel grains in the micro-app necessitated the need of mesh elements smaller than the size of a fuel grain. A grid of equidistant unit cells was created, having a pitch of 0.0489 cm, and consisted of a spherical fuel grain of diameter 0.0044 cm surrounded by graphite moderator thus preserving the C:U ratio per unit cell. Unfortunately, an entire reactor fuel block could not be modeled heterogeneously using these microscopic unit cells. Therefore, setting the boundary conditions to reflective and adiabatic for cross-section generation and the heat equation, respectively, an infinite reactor is simulated by a single micro-app. The neutron mean free path (MFP) at 1 MeV in room temperature graphite is 4.6 cm; hence, a neutron interacts with the boundary of a micro-app many times during simulations before colliding.

To remove spatial effects in cross-section generation, a homogeneous micro-scale unit cell was provided for cross-section generation only. The homogeneous unit cell contained the exact same number of atoms per isotope as the heterogeneous unit cell. The side length of the homogeneous unit cell was 0.0488 cm.

To illustrate the difference in the models used for the homogeneous versus heterogeneous simulations, the material properties of homogeneous fuel were found in the literature and were different from the material properties of the heterogeneous materials. Table I lists the values and sources of each material property.

Table I. Material Properties: Material properties for both the homogeneous and heterogeneous models.

Property	Homogeneous	Heterogeneous	Source
Fuel Density (kg/cm ³)	1.73E-3	1.08E-2	[4], [5]
Fuel Thermal Conductivity (W/cm K)	0.2	1.46E-3	[4], [5]
Fuel Specific Heat (J/kg K)	998	265.862	[4], [5]
Graphite Density (kg/cm ³)	----	1.67E-3	[5]
Graphite Thermal Conductivity (W/cm K)	----	1.05	[5]
Graphite Specific Heat (J/kg K)	----	1256.04	[5]

3.2. Macro-App Domain

The macro-app consists of a highly simplified representation of TREAT as a single homogenous fuel cube surrounded by a pure graphite reflector. The fuel cube has a side length of 135.17 cm, centered in a cube of reflector with a side length of 260.59 cm. The boundary conditions outside the reflector are adiabatic and vacuum for the heat equation and neutron diffusion equation, respectively. The homogeneous fuel meat properties are found in Table I with the reflector properties coming from the graphite properties provided in the last three rows of the “Heterogeneous” column.

The macro-app is similar to the TREAT reactor only in terms of fuel meat composition and reflector composition, approximated as a cube. The macro-app does not include any air coolant channels, control rod positions, individual assemblies, or the experiment and slot positions. The simplicity of the macro-app aided in development and comparison of the method to isolate the heat diffusion time lag phenomenon from other effects of more complex geometry domains.

4. CROSS-SECTION GENERATION

A temperature-dependent multi-group cross-section library is necessary to account for temperature changes in the fuel and graphite during a simulated transient. Using an appropriate spectrum, cross-sections were collapsed to two energy groups using the Monte Carlo reactor physics code Serpent 2 [9]. The energy cutoff in MeV between each group was at 2×10^{-6} thus separating the fast spectrum from the thermal spectrum [10].

The YAKXS library format used by MAMMOTH provides the capability to support a pulse transient simulation with temperature-dependent cross-sections. A change in boron content within the graphite at the beginning of the simulation initiates the transient, similar to control rod removal in TREAT. The library consists of state or grid points. Each grid point indexes a specific boron concentration and a specific temperature. Each grid point represents a single computational simulation in Serpent 2, in which a single temperature state for each bulk material and boron content were assumed. Table II provides the atomic fractions of isotopes for the heterogeneous and homogeneous models for Serpent 2 for both the “rod in” and “rod out” configurations of boron. “Rod in” is the state before the transient and “rod out” is the state just after the transient has begun.

Table II. Atomic Fractions: Atomic densities ($\times 10^{24}/\text{cm}^3$) for cross-section generation with Serpent 2 [11].

Isotope	Homogeneous		Heterogeneous	
	Rod In	Rod Out	Rod In	Rod Out
⁵⁴ Fe	2.91144E-7	2.91144E-7	2.90157E-7	2.90157E-7
⁵⁶ Fe	4.57034E-6	4.57034E-6	4.55484E-6	4.55484E-6

⁵⁷ Fe	1.05549E-7	1.05549E-7	1.05191E-7	1.05191E-7
⁵⁸ Fe	1.40467E-8	1.40467E-8	1.39990E-8	1.39990E-8
⁵⁰ V	1.53386E-9	1.53386E-9	1.52866E-9	1.52866E-9
⁵¹ V	6.12011E-7	6.12011E-7	6.09936E-7	6.09936E-7
¹⁰ B	1.69526E-7	1.13145E-7	1.69142E-7	1.12761E-7
¹¹ B	6.82363E-7	4.55424E-7	6.80818E-7	4.53879E-8
Graphitized ¹² C	0.05086641	0.05103951	0.05086641	0.05086641
¹² C	0.03534784	0.03546813	0.03534784	0.03534785
²³⁴ U	8.50518E-8	8.50518E-8	0.00022150	0.00022150
²³⁵ U	8.71445E-6	8.71445E-6	0.02269540	0.02269540
²³⁶ U	4.09370E-8	4.09370E-8	0.00010661	0.00010661
²³⁸ U	5.05918E-7	5.05918E-7	0.00131758	0.00131758
¹⁶ O	1.86927E-5	1.86927E-5	0.04868220	0.04868220

The homogeneous unit cell grid points were then compiled into a cross-section library dependent on the temperature of the fuel meat and boron concentration. The heterogeneous unit cell grid points were compiled into a cross-section library dependent on the grain temperature, moderator temperature, and boron concentration.

5. SIMULATION METHOD

To produce comparable temperature controlled transients, the neutron diffusion and heat diffusion equations were coupled to produce the temperature feedback using the cross-section libraries. The MOOSE MultiApp system was set to transfer power density to the heat equation simulations on the unit cell domain at 27 positions in a 1/8th reflected block simulation domain of the neutron diffusion equation; this being the macro-app. The power density was computed from the neutron flux solution on the macro-app. The 27 micro-app simulations generated all the heat in the fuel grain and then solved for the average temperature of the graphite and fuel grain. The average temperatures were then transferred to the macro-app with temperature values between micro-app positions being interpolated. The solution on all domains converged with multiple transfers before proceeding to the next time step.

An eigenvalue solution of the macro-app with all material held at 300 K and the boron concentration being set to the “rod in” state was used as the initial condition for the transient simulation. The boron was changed to the “rod out” state in 0.005 seconds at the very beginning ($t = 0$ s) of the transient simulation. The boron state was left unchanged for the rest of the simulation ending at 2 seconds.

MAMMOTH provides many different computation options. A backwards Euler scheme was applied to time integration. First order Lagrange elements were used in the spatial meshes. The computation method was 1st order in time and 2nd order in space. Picard iterations insured convergence on the current time step before moving to the next time step.

Because MAMMOTH is a modular code, transfers and feedback were altered to explore the effects on the transient pulse. The MultiApp system allows for micro-apps to be swapped easily between the homogeneous unit cell and the heterogeneous unit cell. Swapping micro-apps allowed the alteration of feedback temperatures supplied to the cross-section library. The homogeneous (HO) model used the homogeneous cross-section library dependent only on one feedback temperature, $S_{HO} = f(T^*)$, representing the fuel mixture temperature of a unit cell. The heterogeneous (HT) model used the

heterogeneous cross-section library depended on the two feedback temperatures, $S_{HT} = f(T_{fg}^*, T_m^*)$, representing the fuel grain temperature and moderator temperature of a unit cell.

To provide a single cross-section to the macro-app, a simple volume weighting of the HT model was able to collapse the heterogeneous unit cell cross-sections due to the neutron flux being the same throughout the micro-app domain, both in the moderator and fuel grain. This assumption of a “flat” flux from one boundary to the other in the micro-app was proven to be true with Serpent 2 flux tallies.

Feedback temperatures were taken from the micro-app simulations of either homogeneous or heterogeneous unit cells. The mixture temperature, T_{mix} , was from the homogeneous unit cell. Both reference cases used the mixture temperature. This assumed the heat was deposited directly into the fuel mixture eliminating any time lag.

The heterogeneous unit cell micro-app simulation assumed all the fission energy was deposited into the fuel grain. The energy then diffused into the moderator. The micro-app could transfer the fuel grain temperature, T_{fg} , and moderator temperature, T_m , to the macro-app. Table III summarizes the five MAMMOTH simulation used to test assumptions and explore the time lag phenomenon.

Table III. MAMMOTH Simulation Cases: Summary of MAMMOTH simulations specifying feedback temperatures.

Simulation Case	Cross-Section Library Model	Micro-app Unit Cell Type
A	$S_{HO}(T_{mix})$	Homogeneous
B	$S_{HT}(T_{mix}, T_{mix})$	Heterogeneous
C	$S_{HO}(T_m)$	Homogeneous
D	$S_{HT}(T_m, T_m)$	Heterogeneous
E	$S_{HT}(T_{fg}, T_m)$	Heterogeneous

To establish comparisons between equivalent transient pulses simulated with each cross-section library, no feedback simulations, where all temperatures were kept fixed at 300 K, were used to match reactor period on both libraries. This reactivity inserted, by changing the boron concentration, for each model was kept constant in all simulations when feedback coupling was applied.

In order to show the phenomenon of time lag due to heat diffusion, a reference simulation without the phenomenon must be compared to a simulation exhibiting the time lag. From reference simulations, the changes in values of interest were found. Cases A and B are the two reference cases for each model.

Due to the small amount of ^{238}U , the probability of a neutron being absorbed in resonances before fission is low even with Doppler broadening from the fuel grain temperature, T_{fg} . As such, cases C and D take advantage of this assumption. Case E tests the assumption of the feedback being dominated by the moderator temperature, T_m , by also including the fuel grain temperature, T_{fg} . Cases C and D assumes all feedback temperatures are at the moderator temperature.

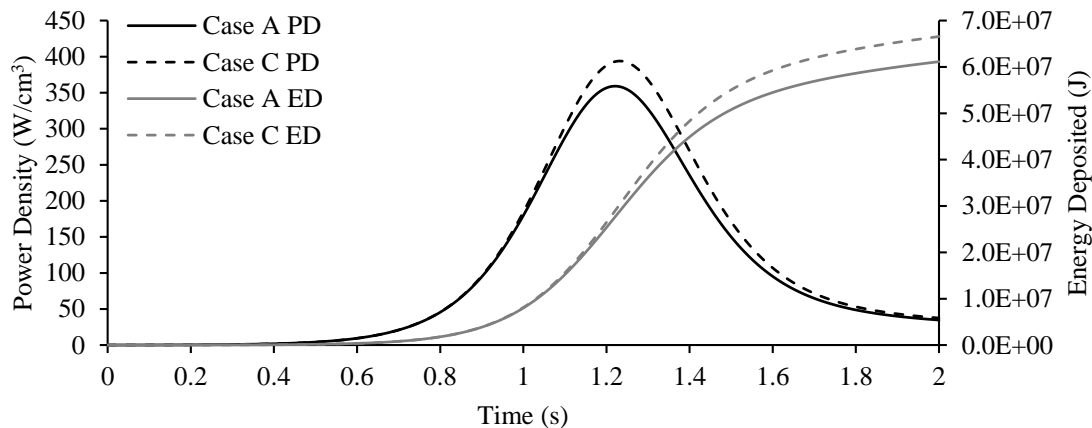
6. MAMMOTH RESULTS

Heat diffusion time lag affects the power behavior of a transient pulse. As such, three parameters of interest were compared from the MAMMOTH simulations. The first value was the average power density of the fueled block surrounded by the reflector labeled “PD” in the figures. The power density was directly related to the number of fission reactions, which was proportional to the scalar flux. The power density was also the value that mainly links the neutron diffusion equation to the heat equation.

The second value of interest was the integrated power or energy deposited into the fueled block, labeled “ED” in the figures. Since TREAT is air-cooled and transient pulses happen quickly, the entire reactor was treated as an adiabatic reactor with no cooling during the transient. Limits were set on the amount of energy that could be generated to prevent damaging the cladding or fuel. Changes in the amount of energy deposited because of heat diffusion time lag would be important as a safety consideration. The macro-app was also treated as an adiabatic reactor so the energy deposited would not leave the simulations.

The third value was the feedback temperatures of the material controlling the pulse. The type of temperature feedback and number of feedback temperatures needed was dependent on the cross-section model used.

Figure 2 shows the HO model results. With simulation case A values being taken as the reference, the peak average power density increased by 9.7 % in simulation case C. The energy deposited increased by 8.8 % at the end of the simulation at 2 seconds. The energy still contained in the fuel grain at 2 seconds had not diffused into the grain, making a comparison of the mixture temperature with the moderator temperature misleading. Figure 2 shows the slight temperature delay as the pulse began and the development throughout the rest of the transient.



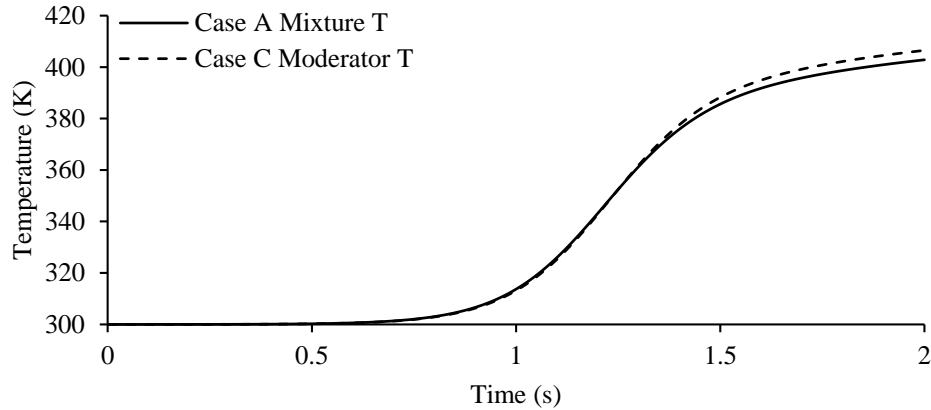
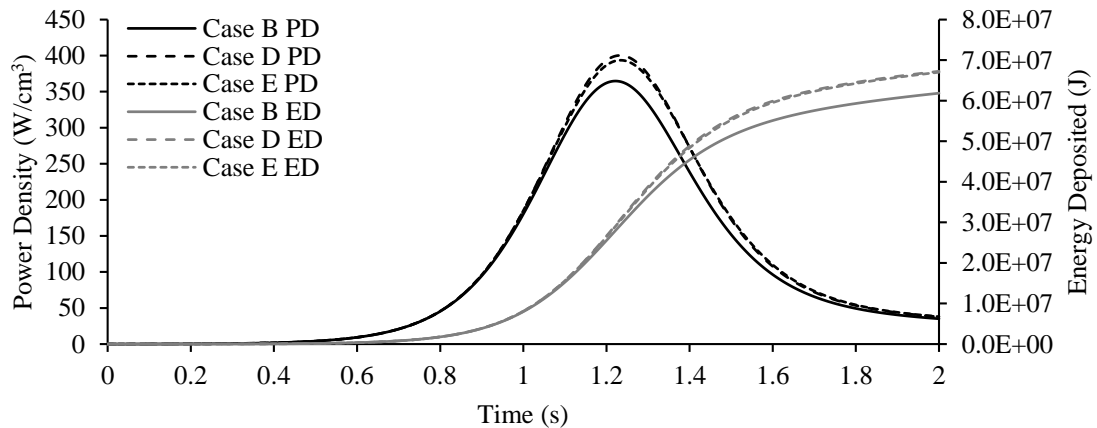


Figure 2. Homogeneous unit cell cross-section library MAMMOTH simulation results.

Figure 3 shows the HT model results. Values from simulation case B served as the comparison reference. The peak average power density increased by 9.7 % for simulation case D and 7.9 % for simulation case E. The energy deposited increased by 8.7 % for case D and 8.3 % for case E. The grain temperature spike in figure 3 from case E also happened in case D but case D assumed the fuel grain's contribution to feedback was negligible.



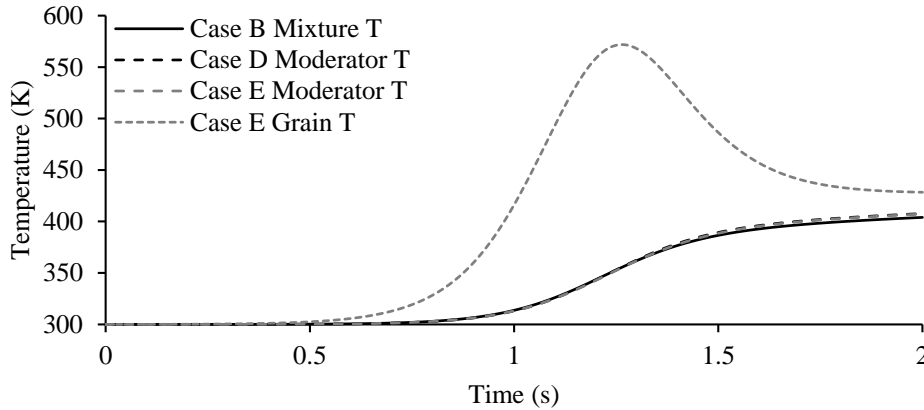


Figure 3. Heterogeneous unit cell cross-section library MAMMOTH simulation results.

7. DISCUSSION

The heat diffusion time lag is apparent when examining the increasing portion of the pulse. Figure 4 shows the area of interest for HT model simulations. The moderator temperature from simulation case D and case E is lower than the mixture temperature reported from simulation case B [5]. Due to the feedback being less and more energy being deposited, the temperature values cross and the moderator temperature of case D and case E ends above the mixture temperature of case B, as seen in Figure 3. These trends are also seen in the HO model simulations.

The change in peak power density and the power reduction portion of the transient is responsible for the change in energy deposition due to time lag. Not only does the peak power density change in value, but it also changes slightly in time. The increase in energy deposition increases the temperature of the moderator, but the specific heat of graphite limits the effects to small temperature increases.

Comparisons between simulations using the same model isolated the effects of the time lag. The similar percentage increases in peak power density and energy deposition within both models suggest that the time lag behaves the same in both models. Comparison of the results from all groups suggests that there is a slight difference due to the homogenization method of the cross-sections. Figure 5 illustrates the change in peak average power density. A 1.6 % increase of peak power density for case B occurs from case A. The corresponding energy deposition increases by 1.2 %. Simulation case D increases peak power density by 1.6 % and increases energy deposition by 1.1 % from simulation case C.

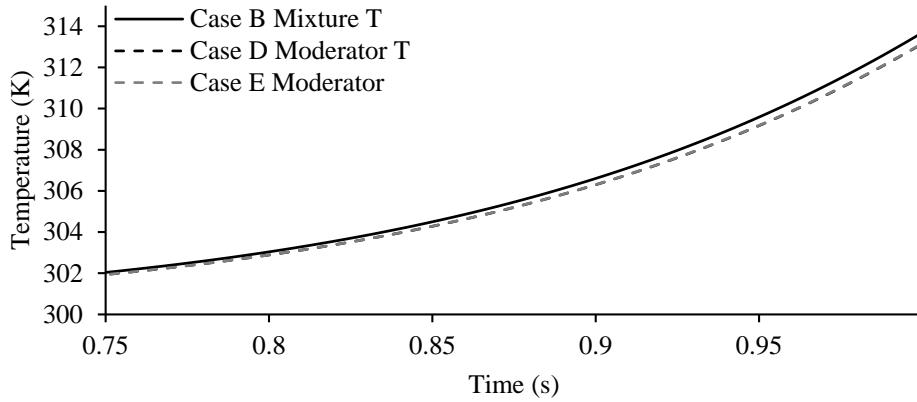


Figure 4. Heterogeneous library moderator temperatures showing the heat diffusion time lag.

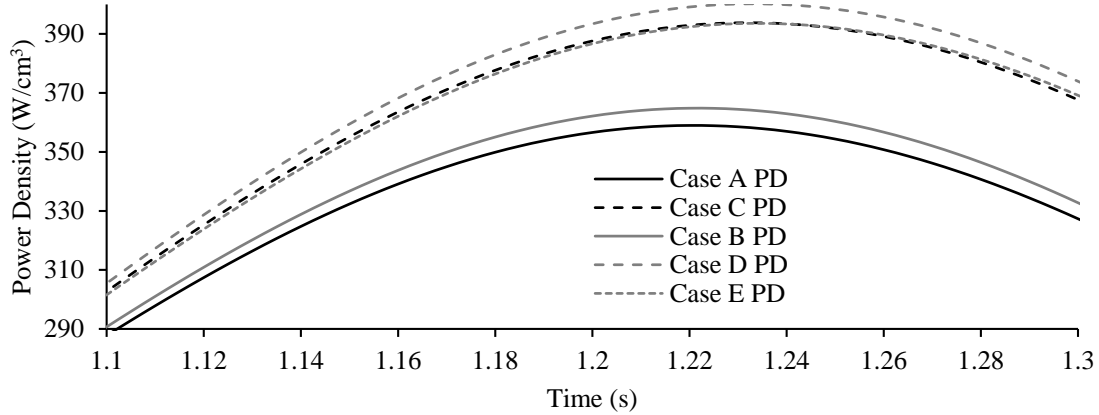


Figure 5. Comparison of average peak power densities.

The inclusion of both temperatures, the grain and moderator temperatures, of simulation case E slightly lowers the peak power density and energy deposited from simulation case D. The behavior suggests the heat diffusion time lag is not entirely dependent on the moderator temperature alone; the temperature of the fuel grain also affects the pulse power profile. If the characteristics of the fuel grain were to change, the affect on the pulse power profile would also vary. A decrease in the enrichment would change the Doppler broadening impact on the fission cross-section for ^{235}U and the absorption cross-section for ^{238}U . The simulation method to handle multiple unit cell material feedback temperatures is not possible with the cross-section library of the HO model.

8. CONCLUSION

The MOOSE-based reactor physics tool MAMMOTH has been applied in simulations of a temperature limited transient pulse to illustrate the phenomenon of heat diffusion time lag. The simulations coupled the heat equation and neutron diffusion equation from different domain sizes through the MOOSE MultiApp system. The macro-app was a reflected homogeneous block of fuel similar to the TREAT

reactor fuel. Multiple micro-app simulations were spread throughout the macro-app. The micro-app was a UO_2 spherical grain suspended in a graphite matrix. Power density was transferred from the macro-app simulation to the micro-app simulations. The average temperatures of the grain and moderator were transferred from the micro-app creating a field of temperature values in the macro-app simulation.

Temperature-dependent cross-sections, generated on two different unit cell configurations, provided the mechanisms for both initiating the pulse and for temperature feedback. Both configurations contained the same number of atoms per isotope. The difference was the location of atoms within the unit cell. The heterogeneous unit cell was the same as the micro-app. The cross-section library from the micro-app was a function of boron concentration, moderator temperature, and grain temperature. The homogeneous unit cell cross-section library was a homogeneous mixture of all isotopes found in the heterogeneous unit cell and was a function of boron concentration and fuel mixture temperature. Both libraries separated cross-sections into two energy groups to divide thermal neutrons from fast neutrons. The actual feedback temperature provided to the libraries was varied depending on the desired source of temperature feedback.

By varying the source of temperature and library, the effect of diffusion time lag on the beginning, peak, and end of the temperature limited pulse was simulated with MAMMOTH. Both libraries were able to produce the time lag effect. The heterogeneous unit cell library was able to show the effect on the pulse when the grain temperature was different from the moderator temperature.

Comparison of the two cross-section simulation models showed differences smaller than those produced by the time lag within the model. The time lag percent changes within each library model were consistent with the percent changes in the other library model.

Future work with this method of simulating time lag transient pulses includes temperature-dependent properties, expansion of energy groups to better represent neutron behavior in the reactor, and macro-app geometries matching the TREAT configuration. The method would not change significantly with these improvements; only the computational requirements would increase and the results would have greater fidelity.

Future simulations with lower enrichments of ^{235}U are of particular interest for future work as the feedback mechanism changes with enrichment. Lower enrichments usually mean an increase in ^{238}U as more uranium is put in the reactor. The moderator to fuel grain ratio would change. The Doppler broadening increasing resonance capture of more ^{238}U would move the feedback from being dominated by the graphite moderator temperature to a more mixed feedback mechanism. The time lag method developed with MAMMOTH already handles multiple material feedback temperatures, provided the heterogeneous unit cell cross-section library is applicable.

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