Heat Source Characterization in a TREAT Fuel Particle Using Coupled Neutronics-BCMC Calculations

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INTRODUCTION

The Transient Test Reactor (TREAT) reactor that is currently being prepared for restart at Idaho National Laboratory [1] is an air-cooled, thermal, graphite-moderated reactor for testing of nuclear fuels under severe accident conditions. The TREAT fuel assemblies are made up of a macroscopically homogeneous mixture of highly enriched uranium and graphite. Microscopically, fuel grains of unknown shape with a maximum diameter estimated at 44 μm [2] are dispersed in a graphite matrix with an unknown, yet usually assumed uniform, spatial distribution. The local temperature distribution is affected by the fission heating source term that is neither uniform nor restricted to the fuel. While fission fragments deposit the majority of their energy in the fuel, some energy is indeed deposited in the graphite. Other recipients of fission energy, namely photons or electrons, feature larger mean free path lengths leading to a uniform distribution of energy. An effort is currently underway to replace the TREAT highly enriched uranium (HEU) core with a low enriched uranium (LEU) core. While the detailed temperature distribution around a fuel grain is insignificant for the HEU core's behavior, it is essential for understanding the LEU core's thermal feedback. The focus of this work is the characterization of the heat source around a TREAT fuel grain.

Currently, TREAT's primary feedback mechanism is spectral shift: an increase of temperature shifts the Maxwellian distribution of thermal neutrons to higher energies; on average neutrons see smaller fission cross sections (due to their $1/v$ dependence) and predominantly get absorbed or leak from the core leading to a negative feedback [3]. In the HEU core, the feedback is relatively slow and dominated by the graphite temperature, while the LEU core also features instantaneous Doppler feedback that is governed by temperature of the fuel. Therefore, for accurate prediction of the LEU core's behavior, a detailed knowledge of the local temperature distribution is required.

Previous work by Mo [2] uses the one-dimensional binary-collision Monte-Carlo code (BCMC) SRIM [4] for computing the damage region around a TREAT fuel grain for assessing the thickness of the damage region and resulting degradation of thermal conductivity using 100 MeV xenon projectiles. Mo then computes the temperature distribution during a transient using COMSOL [5] taking into account the damage region, but restricting the heat source to be uniform within the fuel grain. This work expands on Mo's effort by more accurately characterizing the heat source term. Future work will elaborate on the distribution of the radiation damage around the fuel grain after a certain number of transients.

In this work we use use the Magpie application that is based on the Multiphysics Object-oriented Simulation Environment (MOOSE) [6]. Magpie allows tight coupling of finite element method (FEM) based codes and microscale codes such as the three-dimensional BCMC code MyTRIM [7]. This new capability allows an online computation of radiation damage and fission product energy deposition coupled with heat conduction, neutronics, and species diffusion when embedded in the MAMMOTH multiphysics app [8]. In the summary, heat sources around a fuel grain are computed for the HEU core, even though the target application of this analysis is the LEU core: the fuel specified in both the neutronics and micro-structure model is HEU fuel containing mostly U-235. Even though we believe the general conclusions about the shape of the heat source will be similar, the final paper will include numerical results for LEU fuel.

MULTIPHYSICS MODELING OF TREAT FUEL PARTICLE

For modeling the dynamic behavior of a TREAT fuel grain, the macroscopic model comprises the time-dependent neutron diffusion equation coupled with the heat-conduction equation. At selected points within the domain we obtain fission rates separated by energy group and nuclide that are used to sample primary knock-on atoms (PKAs). A binary collision Monte-Carlo model is used to compute the energy deposition of the fission fragments serving as a source term for the microscopic heat conduction problem. This section details the models utilized within this work.

Coupled Transient Neutron Diffusion Model

The time-dependent, multigroup neutron diffusion equation is given by:

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} - \nabla D_g(\vec{r},T)\cdot\nabla\phi_g(\vec{r},t) + \Sigma_{r,g}(\vec{r},T)\phi_g(\vec{r},t)$$
$$= \sum_{g'=1,g'\neq g}^{G} \Sigma_s^{g'\to g}(\vec{r},T)\phi_{g'} + (1-\beta_g)\frac{\chi_{p,g}}{k}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(\vec{r},T)\phi_{g'}$$
$$+\chi_{d,g}\sum_{i=1}^{6}\lambda_i C_i(\vec{r},t)\ g=1,..,G, \quad (1)$$

where g is the energy group index, ϕ_g is the scalar flux of energy group g, C_i is the delayed neutron precursor concentration of delayed precursor group i, T is the temperature, v_g is the neutron speed in group g, D_g is the diffusion coefficient in group g, $\Sigma_{r,g}$ is the removal cross section, $\Sigma_s^{g' \to g}$ is the scattering cross section from group g' to g, β is the delayed neutron fraction, $\chi_{p,g}$ is the prompt fission spectrum, k is the eigenvalue whose meaning in transient calculations will be explained later, $\nu\Sigma_f$ is the fission neutron production cross section, $\chi_{d,g}$ is the delayed neutron spectrum, and λ_i is the decay constant of precursor group i. The neutron diffusion equation is augmented by the delayed neutron precursor equations:

$$\frac{\partial C_i}{\partial t} = \beta_i \sum_{g'=1}^{G} \nu\Sigma_{f,g}(\vec{r},T)\phi_g - \lambda_i C_i(\vec{r},t),\ i = 1,..,6, \quad (2)$$

where β_i is the delayed neutron fraction in delayed group i. Finally, the heat equation determines the distribution of temperature in the TREAT model and is given by:

$$\frac{\partial(\rho c_p(T)T)}{\partial t} - \nabla k(T)\cdot\nabla T = \sum_{g=1}^{G} \kappa\Sigma_{f,g}\phi_g, \quad (3)$$

where ρ is the density, c_p is the specific heat capacity, and k is the heat conduction coefficient . The heat conduction equation is solved only in the fuel region, because outside of it heat-sources are absent and the short duration of the transient does not allow a significant increase in temperature through conduction from the fuel region. The temperature outside the fuel region is kept isothermal at $T = 300$ K. The temperature dependence of c_p and k is given by a polynomial fit of third and second order, respectively that will be stated in the full paper.

Initial conditions for Eqs. (1) through (3) are obtained by solving an eigenvalue problem coupled with a steady state heat conduction equation. The initial scalar fluxes, temperatures and the eigenvalue are transferred and used to set the corresponding values for the transient calculation at $t = 0$. The computed eigenvalue of $k = 0.9909304$ is applied in Eq. (1) throughout the entire transient so that without any other changes, the system is in a forced steady-state. The transient is initiated at $t = 0$ by control rod withdrawal that is modeled by boron dilution.

Information Transfer from Macroscale to Microscale

At each timestep, a micro-structure calculation is performed for a selection of points. In this abstract results are only presented for a point located at the center of the TREAT core. For each point, we transfer two quantities to the microstructure calculation: (1) a probability density function (pdf) for sampling the fissioning nuclide and the energy group of the neutron causing fission, and (2) the power that is generated within the considered micro-structure domain. The partial fission rate pdf is discussed along with the sampling process for PKAs in the next section. Let the volume of the fuel grain of interest and the core power density be denoted by V_f and $p(\vec{r},t)$, respectively. Then the total power $P_f(t)$ that is generated within a fuel grain centered at $\vec{r}_f$ is approximately given by:

$$P_f(t) \approx p(\vec{r}_f,t)\frac{V_f}{f}, \quad (4)$$

where the fuel volume fraction $f = 1:2571 \approx 0.0004$ [2].

Primary Knock-on Atoms produced by Fission

The distribution of fission fragments' atomic and mass number, energy and direction of motion is sampled based on the solution from neutronics calculations. For this purpose, the partial fission rate of target isotope i denoted by $F_i(\vec{r},E)$ is defined as:

$$F_i(\vec{r},E,T)dE = N_i(\vec{r})\sigma_{f,i}(\vec{r},E,T)\phi(\vec{r},E,t), \quad (5)$$

where N_i is the number density of isotope i, and $\sigma_{f,i}$ is the microscopic fission cross section of isotope i. Within the multigroup formalism, the definition of the partial fission rates becomes:

$$F_{g,i} = N_i(\vec{r})\sigma_{f,g,i}(\vec{r},T)\phi_g(\vec{r},t), \quad (6)$$

where g is the energy group, and i is the target isotope. We define the normalized, discrete pdf $\pi(i,g)$ of a fission event being caused by neutron in group g interacting with nuclide i. The pdf can be computed as:

$$\pi(i,g) = \frac{F_{g,i}}{\sum_{g=1}^{G}\sum_{i=1}^{I}\Delta E_g F_{g,i}}. \quad (7)$$

The marginal distribution $\pi(i)$ is obtained by summing over all energy groups:

$$\pi(i) = \sum_{g=1}^{G}\pi(i,g). \quad (8)$$

A cumulative probability density function (cdf) $\Pi(i)$ can be computed from this marginal distribution by:

$$\Pi(i) = \sum_{j=1}^{i}\pi(i). \quad (9)$$

The cdf $\Pi(i)$ is sampled to determine the target isotope denoted by i^*.

Given a sampled target isotope, $i = i^*$, a conditional distribution, $\pi(g|i^*)$ is obtained from which we compute the conditional cdf $\Pi(g|i^*)$:

$$\Pi(g|i^*) = \sum_{g'=1}^{g}\Delta E_{g'}\pi(g'|i^*), \quad (10)$$

that is used for sampling the group index g^*. A continuous value for the energy E^* is then sampled uniformly between the energy bounds $[E_{g^*+1}, E_{g^*}]$.

Using the fissioning target isotope and energy of the neutron causing fission, ENDF fission yield data [9] is used for determining the fission fragments' mass and atomic number. An empirical relationship is applied to obtain the fission fragments' energy and momentum. The following assumptions are made throughout:

- We neglect rare three fission fragments.
- The fission process is isotropic in the lab frame.
- Momentum of the fission inducing neutron is neglected.
- Momenta of the fission product neutrons are neglected.

ENDF fission yield data is separated by the energy of the neutron causing fission into thermal, epithermal, fast and high data sets. We divide the energy range as follows:

Thermal:	≤ 0.5 eV
Epithermal:	0.5 eV $<$ E $\leq$ 0.75 MeV
Fast:	0.75 MeV $<$ E $\leq$ 7 MeV
High:	$>$ 7 MeV

Based on E^* and i^* the correct ENDF data is retrieved that essentially contains probability density functions $Y(Z, A)$. The normalized marginal and conditional probability density functions $\lambda(Z)$ and $\lambda(A|Z^*)$ are obtained as:

$$\lambda(Z) = \frac{\sum_A Y(Z, A)}{\sum_A \sum_Z Y(Z, A)}$$
$$\lambda(A|Z^*) = \frac{Y(Z^*, A)}{\sum_A \sum_Z Y(Z, A)}. \quad (11)$$

The corresponding cdfs $\Lambda(Z)$ and $\Lambda(A|Z^*)$ are computed analogous to Eq. (9) and (10), respectively. These cdfs are sampled for the atomic and mass number of the *first* fission fragment denoted by Z_1 and A_1. The mass number of the second product can be determined by invoking conservation of mass:

$$A_2 = A_{target} - A_1 - \bar{\nu} \quad (12)$$

where A_2 is the mass number of the second fission product, A_{target} is the mass number of the target nucleus, and $\bar{\nu}$ is the (integer) number of neutrons released during fission. $\bar{\nu}$ is sampled on the interval of the nearest integers less than and greater than ν and is weighted based on the true value of ν. Similarly, Z can be obtained by invoking conservation of charge:

$$Z_2 = Z_{target} - Z_1 \quad (13)$$

where Z_2 is the atomic number of the second fission product, and Z_{target} is the atomic number of the target.

The average kinetic energy T_{kin} of the fission products can be calculated using the empirical relationship on both Z_{target} and A_{target} of the target isotope [10]:

$$T_{kin} = 0.1178 \frac{Z_{target}^2}{A_{target}^{1/3}} + 5.8 \quad (14)$$

Using an energy and momentum balance the energy of each fission product can be calculated:

$$T_{kin} = E_1 + E_2 \quad (15)$$
$$\vec{p}_1 = \vec{p}_2 \quad (16)$$

Solving for the energy of each fission product gives:

$$E_1 = T_{kin} \left(1 + \frac{A_1}{A_2}\right)^{-1} \quad (17)$$
$$E_2 = \frac{A_1}{A_2} E_1 \quad (18)$$

The direction of motion of the first fission product will be sampled uniformly on the unit sphere and the second fission product travels in the opposite direction.

Binary Collision Monte Carlo and Fission Product Heat Deposition

The binary collision approximation simulates the trajectory of ions through matter by assuming that it experiences a sequence of indepentent, binary collisions with the host atoms [4]. For computing the present host material composition and density, the number densities of the present isotopes are represented as FEM grid functions. For convenient use in MyTRIM, the average of the concentrations over each FEM element is computed in a step referred to as rasterization. The position of PKAs and the resulting cascade are tracked on the FEM mesh and nuclear cross sections are retrieved using the averaged compositional data.

The fission fragments cause cascades of follow-on displaced ions. These ions' movement through the micro-structure domain is tracked by MyTRIM and at each collision event the difference between the initial and final energy is deposited in the mesh element where the displaced atom undergoes the collision. In addition, at the location where an ion comes to rest, the binding energy needs to be deposited. The final result is the spatial distribution of fission energy deposition around the fuel grain.

RESULTS AND ANALYSIS

(a) Transient 15 Neutronics model

The TREAT neutronics model has previously been described and used in [11] and will be explained in more detail in the final paper. The model comprises five different regions: fuel, graphite assemblies with Zirconium

cladding, graphite assemblies with Aluminium cladding, permanent graphite reflector, and control rods. A total of 355,712 hexahedral elements are used in this model, and the 11-group diffusion model is discretized using first order Lagrange continuous finite elements. For discretization of time, a constant time step of $\Delta t = 0.1$ seconds is used in conjunction with the Crank-Nicolson time integrator.

(b) UO2 pellet - Graphite model

The micro-structure model comprises three isotopes: ^{12}C in the region outside of the fuel grain, ^{235}U and ^{16}O within the fuel grain. Note that this composition resembles the HEU core, while in the LEU core the majority of uranium will be ^{238}U creating potentially different fission products. The full paper will include LEU results. For avoiding Gibbs' phenomenon when projecting the concentration values onto an FEM mesh, it is essential to ensure a smooth transition of the concentration from one region to another. For this purpose, we use the following expressions assuming a spherical fuel grain:

$$c_j(\vec{r}) = \frac{1}{2}\left(C_{in,j}\,(1+B) + C_{out,j}\,(1-B)\right)$$
$$B = \tanh a\left(\frac{r}{R} - \frac{R}{r}\right), \tag{19}$$

where r is the distance from the centroid of the fuel grain, R is the radius of the fuel grain, and the free parameter a determines the slope of the transition and we select $a = 8$. The parameters $C_{in,j}$ and $C_{out,j}$ are the asymptotic concentrations inside and outside the sphere, respectively. The full paper will generalize the shape of the fuel grain to ellipsoids as it was conjectured that the fuel grain might be shaped more like "corn flakes" [12], [13].

The average minimum distance of two fuel grains can be estimated assuming (1) that the fuel grains are spherical and (2) the fuel is uniformly distributed. Using the fuel volume fraction f we can find that the number of fuel grains in a box of dimension L is roughly:

$$N \approx \left(\frac{L^3 f}{4/3\pi R^3}\right)^{1/3}. \tag{20}$$

Following [14], a rough approximation of the average minimum distance between two grains in a box of dimension L is:

$$< r > \approx \left(\frac{L^3}{N}\right)^{1/3} = \left(\frac{4}{3}\frac{\pi}{f}\right)^{1/3} r \approx 22R. \tag{21}$$

The average minimum distance between fuel grains is much larger than the typically range of fission fragments and hence the domain boundaries are chosen such that fission product cascades are unlikely to reach them.

We are interested in determining the microscopic distribution of the heat source q'''. The graphite volume associated with the fuel grain is denoted by V_g and can be assumed to be given by $V_g \approx V_f/f$. According to Ref. [15] 80% of the fission energy is released as fission fragment and 15% is distributed to recipients that will essentially create a spatially uniform contribution, the leftover 5% are non-revoverable. The arbitrarily normalized shape of the fission fragment energy distribution is denoted by $\tau(\vec{r}, t)$. We write q''' as

$$q'''(\vec{r}, t) = \alpha\tau(\vec{r}, t) + \beta(t). \tag{22}$$

For determining the coefficients α and β we require:

$$P_f(t) = \alpha \int_{V_g} \tau(\vec{r}, t)dV + V_g\beta$$
$$\frac{V_g\beta}{\alpha \int_{V_g} \tau(\vec{r}, t)dV} = \frac{15}{80} = \frac{3}{16}. \tag{23}$$

We finally obtain:

$$q'''(\vec{r}, t) = \frac{p(\vec{r}_f, t)}{1 + 3/16}\left[\frac{V_f}{f}\frac{\tau(\vec{r}, t)}{\int_{V_g} \tau(\vec{r}, t)dV} + \frac{3}{16}\right]. \tag{24}$$

Numerical Results

We consider a spherical fuel particle of radius $r = 20\mu m$ located at the center of the transient 15 TREAT core [11]. The heat source depicted in Fig. 1 is a snap shot at roughly $t = 2$ seconds into the transient putting it close to the peak power. Figure 1 depicts averages over spherical shells centered about the fuel grain's center. At the selected time TREAT's total power is 312 MW and the macroscopic power density at the selected point is $p(\vec{r}_f, t = 2) = 262.9$ W/cm^3. The microscopic distribution of power is highly concentrated in the fuel grain reaching 0.5 MW/cm^3 and a significant fraction of the energy is deposited within a distance of 10 μm of the fuel grain in the graphite matrix. The reason for the large power density is that the fuel grain only assumes a very small fraction of the total volume, but receives most of the energy deposition from fission fragments. As we move away from the center of the fuel particle, the asymptotic value of the heat source is $\lim_{r\to\infty} q''' = 41.5$ W.

The fit of the heat source in the fuel uses an even polynomial of fourth order, and the moderator power uses a complete fourth order polynomial. The choice of the polynomial in the fuel originates from the observation that the heat source should be symmetric about $r = 0$. As the volume for small r is significantly smaller than for large r the corresponding data points exhibit strong statistical fluctuations.

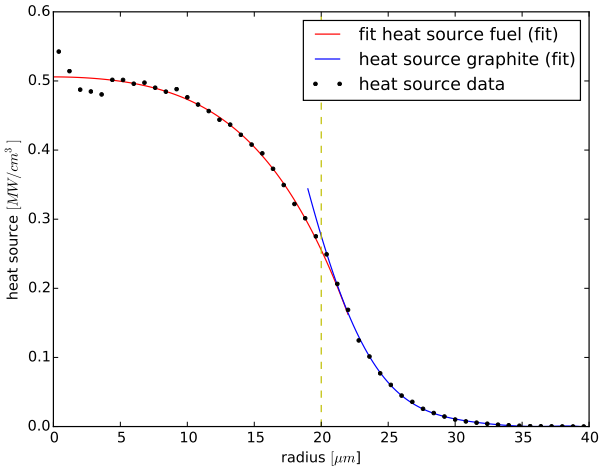

Fig. 1 Heat source for a spherical fuel particle of radius $r = 20\mu m$ at the center of the TREAT transient 15 core at a total power of 312 MW.

CONCLUSIONS AND FUTURE WORK

Within this work we describe a first step of multi-scale, multi-physics modeling of TREAT with particular emphasis on the behavior of the LEU core. We use a BCMC model that is coupled to an FEM application by the Magpie application to characterize the heat source of the micro-structure heat-conduction problem. The BCMC is driven by a macroscopic Rattlesnake [16] neutronics calculation of TREAT transient 15. ENDF fission yield data is utilized for sampling PKAs. We present the shape of the heat source for a spherical fuel grain demonstrating that it significantly deviates from both a uniform distribution and a uniform distribution within the fuel grain and zero outside. The full paper will include results for the LEU core, investigate the effect of the shape of the fuel grain on the heat source, and use the heat source in a transient heat conduction calculation. Future work will include the estimation of the damage region within and around a fuel grain after a number of transients taking into account annealing and feedback of the microstructure calculation to the macroscopic neutronics calculation for the LEU core.

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