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Numerical Method Improvements in Griffin for Pebble Bed Reactors with a Focus on the Computation of Burnup

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ABSTRACT

Griffin, a MOOSE (Multiphysics Object-Oriented Simulation Environment) based application targeting transient multiphysics modeling of advanced reactors, has been used recently to model both high-temperature gas-cooled and fluoride-salt-cooled pebble bed reactors (PBRs). Griffin uses deterministic methods for solving neutron transport and an Eulerian approach to model pebble movement. An Eulerian approach is also used to directly compute burnup instead of using a pass approach like other tools such as VSOP or PANGU. This work discusses verification efforts and numerical method improvements related specifically to the Eulerian modeling approach implemented for directly computing pebble burnup.

Keywords: pebble bed reactor, griffin, verification, burnup

1. INTRODUCTION

Griffin [1] is a MOOSE (Multiphysics Object-Oriented Simulation Environment) [2] based application targeting transient multiphysics modeling of advanced reactors. It includes features for modeling pebble bed reactors (PBRs) and has been used to model both high-temperature gas-cooled and fluoride-salt-cooled PBRs. The modeling approach used by Griffin for equilibrium core calculations is described in detail by Schunert, et. al. [3] and reviewed in this work in the next section. Griffin has also recently been used for multiphysics running-in simulations as described by Hanophy et. al. [4]. This work addresses only the streamline-based modeling approach described in the next section. It is noted that there is a different modeling approach available in Griffin called Pebble Transport Tracking (PTT) [1] that resolves each pebble in the core, however, this approach is still under development.

Efforts are ongoing to verify the modeling approach used by Griffin both for equilibrium and running-in calculations. These efforts have had two main components, basic verification of numerical methods through techniques such as convergence studies, and verification of the overall modeling approach by comparing against Monte Carlo based simulation tools. This article focuses on the former, and specifically on details related to the numerical methods used by Griffin for computing pebble burnup. As described in the next section, Griffin explicitly computes pebble burnup, instead of using a pass based approach like other tools such as VSOP (Very Superior Old Programs) [5] or PANGU (physical analysis code of general utility) [6]. In those codes, burnup is determined though some algorithm that determines the number of times a pebble has passed through the core and correlating that to burnup. Explicitly computing burnup is a useful and unique feature of Griffin, allowing pebble discharge and recycle criteria to be input into the code based on a burnup limit in a more straight forward way. Additionally, the distribution in burnup of pebbles as they exit

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the reactor can also be easily examined since it is explicitly computed. Section 1.1 reviews the modeling approach used by Griffin. The numerical method improvements investigated in this article are described in Section 1.1.1. Results from the new numerical method are shown in Section 2 along with a summary of the verification efforts that originally motivated the implementation of the new numerical method.

1.1. STREAMLINE BASED MODELLING APPROACH

To model a PBR, the assumption is first made that the velocity field for all pebbles can be described well with only several pathlines. The term streamline is used in Griffin for these pathlines and streamline will be used to mean pathline subsequently in this work. A simple example of streamlines in a Griffin model is shown in Figure 1. In this figure, the mesh is used for the neutronics calculations. The scalar flux is moved from the mesh to each streamline in a conservative way in Griffin and the streamlines are used to compute pebble depletion as described next.

Along a streamline, two conserved quantities are computed. The first is $n_c(t, s, \tau)$ which is the volume fraction of pebble type c at time t at streamline coordinate s with burnup τ. To summarize, $\sum_c^C \int_0^\infty n_c(t, s, \tau) d\tau = 1 - \zeta(s)$ where $\zeta(s)$ is the porosity and C is the total number of pebble types. The second quantity, $\vec{N}_c(t, s, \tau)$, are the nuclide number densities for the pebbles with t, s, and τ having the same meanings as before. The balance equations for the conserved quantities are shown in Eq. 1 and Eq. 2 where u is the velocity, a is the streamline area, and p is the power experienced by the pebble. $A(\phi(t, s), \tau)$ is the decay and transmutation matrix that depends on the scalar flux ϕ.

$$\frac{\partial n_c(t, s, \tau)}{\partial \tau} = \frac{-1}{a(s)} \frac{\partial u(s, t) a(s) n_c(t, s, \tau)}{\partial s} - \frac{\partial p_c(t, s, \tau) n_c(t, s, \tau)}{\partial \tau} \tag{1}$$

$$\frac{\partial \vec{N}_c(t, s, \tau)}{\partial \tau} = \frac{-1}{a(s)} \frac{\partial u(s, t) a(s) \vec{N}_c(t, s, \tau)}{\partial s} - \frac{\partial p_c(t, s, \tau) \vec{N}_c(t, s, \tau)}{\partial \tau} + A(\phi(t, s), \tau) \vec{N}(t, s, \tau) \tag{2}$$

This work focuses only on equilibrium core calculations. Griffin uses a direct method for equilibrium core calculations (the methodology used for running-in is discussed in Ref. [4]). The time derivative is set to zero and the equations solved directly. Boundary conditions for the two equations are discussed in Ref. [3]. As it is particularly relevant to this work, it is noted that the inlet and outlet of the streamlines are usually coupled in simulations because some pebbles that exit the reactor will be recycling back into the top of the reactor. Whether a pebble exiting the reactor is recycled back to the top or discarded and replaced with a fresh fuel pebble depends on its burnup being below or above some burnup limit which is set by a user. The equations are solved iteratively within Griffin by breaking the dependency of the inlet flow on the outlet flow by using the outlet flow from a previous iteration and repeating the procedure iteratively until the outlet flow stops changing.

For running-in simulations, there are at least several different pebble types; inert graphite pebbles, starting fuel (lower enrichment), and the equilibrium fuel (higher enrichment). However, this work focuses on equilibrium core calculations where usually only one pebble type is considered; the equilibrium fuel. The c index will thus be dropped in subsequent equations and subscripts won't denote a type of pebble.

An Eulerian approach is used to discretize the balance equations. Each streamline is discretized into M segments. As described in more detail by Schunert, et. al. [3], Griffin initially only included a finite difference (FD) discretization with upwinding for the $\partial/\partial s$ and $\partial/\partial \tau$ terms. As mentioned previously, a key feature of Griffin is that it calculates burnup explicitly instead of tracking pebble passes. This is done by first discretizing burnup space, from zero to some maximum value of interest, into discrete bins. The term bin is used in burnup space simply to distinguish from physical spatial cells. Again, FD is used with

upwinding to discretize the equation in burnup space and handle the $\partial/\partial\tau$ term. The key point about the burnup computation is that the pebbles "advect" through burnup space like they do through physical space. The pebbles "advect" with an analogous velocity that is the power they experience.

1.1.1. Improved Numerical Method for Computing Burnup

The Discontinuous Galerkin (DG) finite element method (FEM) is being investigated for use in place of the simple FD method. Initially, the focus is on burnup space discretization. This work will discuss a mixed discretization with DG-FEM used in burnup space and FD in physical space. Burnup space is discretized into bins with an index h, each bin starting at τ_h with width $\Delta\tau_h$ and $v(\tau)$ is a function that is continuous within bin h, but is allowed to be discontinuous on the boundaries of bins.

Eq. 3 shows the DG-FEM formulation for pebble volume fractions where $n_m(\tau)$ is the pebble volume fraction in the m-th cell of the streamline and can be written $n_m(\tau) = \sum n_{m,j} v_j(\tau)$ where $n_{m,j}$ are coefficients. V_m is the volume of cell m. τ_h^- and $(\tau_h + \Delta\tau_h)^-$ indicate these burnup values approaching from lower burnup. The nuclide number densities are discretized in the same way as shown in Eq. 4. Note again that the time derivative is set to zero in these equations compared to Eq. 1 and 2 because Griffin uses a direct equilibrium core solution scheme.

$$\begin{aligned}\forall\, i,j : &\int_{\Delta\tau_h} \frac{u_{m-1}a_{m-1}}{V_{m-1}} n_{m-1,j} v_j(\tau) v_i(\tau) d\tau + v_i(\tau_h^-) n_m(\tau_h^-) p_m(\tau_h^-) \\ &= \int_{\Delta\tau_h} \left(\frac{u_m a_m}{V_m} n_{m,j} v_j(\tau) v_i(\tau) - p_m(\tau) v_i'(\tau) n_{m,j} v_j(\tau) \right) d\tau \\ &+ v_i((\tau_h + \Delta\tau_h)^-) n_m((\tau_h + \Delta\tau_h)^-) p_m((\tau_h + \Delta\tau_h)^-)\end{aligned} \tag{3}$$

$$\begin{aligned}\forall\, i,j : &\int_{\Delta\tau_h} \frac{u_{m-1}a_{m-1}}{V_{m-1}} \vec{N}_{m-1,j} v_j(\tau) v_i(\tau) d\tau + v_i(\tau_h^-) \vec{N}_m(\tau_h^-) p_m(\tau_h^-) \\ &= \int_{\Delta\tau_h} \left(\left(\frac{u_m a_m}{V_m} + A_h(\phi_m) \right) \vec{N}_{m,j} v_j(\tau) v_i(\tau) - p_m(\tau) v_i'(\tau) \vec{N}_{m,j} v_j(\tau) \right) d\tau \\ &+ v_i((\tau_h + \Delta\tau_h)^-) \vec{N}_m((\tau_h + \Delta\tau_h)^-) p_m((\tau_h + \Delta\tau_h)^-)\end{aligned} \tag{4}$$

Linear basis functions are investigated in this work. Although Eq. 3 and 4 are written in a general way, they can be solved in a simple matrix free way. The same approach is used when "sweeping" the Sn transport equations. Eq. 3 and 4 represent a logically block lower triangular linear system, it is solved without assembling a matrix, first inverting a block on the diagonal and using forward substitution to solve for the next block. In addition to the DG-FEM method shown above, a simple conservative fixup method is implemented to avoid negative densities and volume fractions during the calculation.

2. BURNUP SPACE CONVERGENCE STUDIES

The model used for this numerical investigation work was created to be complex enough that it is representative of high-fidelity models while still being simple enough to run quickly. It is shown in Figure 1 and consists of three regions. A control rod is inserted 40 cm below the top of the core and five streamlines are used in the core region. A similar model was used for the multiphysics running-in calculations presented in [4]. Constant temperatures are used in the fuel region and reflector region and the model uses a pre-generated multigroup cross section set. Also shown in Figure 1 is the power density of the equilibrium core, which is of a realistic profile.

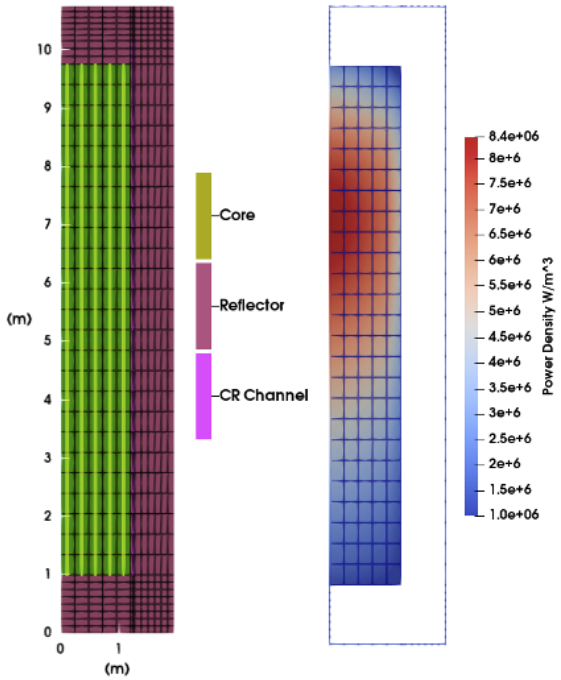

Figure 1. Schematic showing the model used for numerical investigations with the streamlines shown in yellow running through the core region. Also shown is the equilibrium core power density for the model.

A 1.2 pebbles/minute flow rate and assumed burnup limit for the 15.5% enriched fuel pebbles of 136 GWd/tHM is used in this work. The burnup space was discretized from zero to 151 GWd/tHM and numerical experiments were conducted by varying the number of bins used to discretize the burnup space. Results of these studies are presented in the next section.

2.1. BURNUP SPACE CONVERGENCE STUDIES

Figure 2 shows the change in the computed equilibrium core k-eigenvalue value for different numbers of burnup bins. The trend shown for the FD discretization is that the eigenvalue initially increases significantly and then starts the asymptotically approach a value. The multigroup cross section set used in this work was not interpolated on burnup. A clue as to what is causing the behavior seen in the figure is that this behavior does not appear for once through then out (OTTO) cycle calculations. What must then be changing as the burnup grid is refined is the computed volume fraction of pebbles that are discarded and replaced with fresh fuel pebbles.

Figure 3 shows the volume fraction of pebbles with different burnups at the exit of the reactor. Results for 20 and 160 burnup bins respectively are shown and the volume fractions are normalized so that the 20 bin and 160 bin result can be shown on the same scale. Some interesting features can be seen in the results that are highly refined in burnup space. The first peak in volume fraction correlates to pebbles that have experienced one pass when they exit the reactor. There is a second less pronounced peak apparent after the first one which correlates to pebbles finishing their second pass at the reactor exit. Pebbles that have experienced more than two passes have a wider distribution of burnups and peaks are no longer apparent, the general trend is that the volume fraction of pebbles is increasing with increasing burnup. There is a small jump in the pebble volume fractions at the end of burnup space in the high-resolution result. This is because the

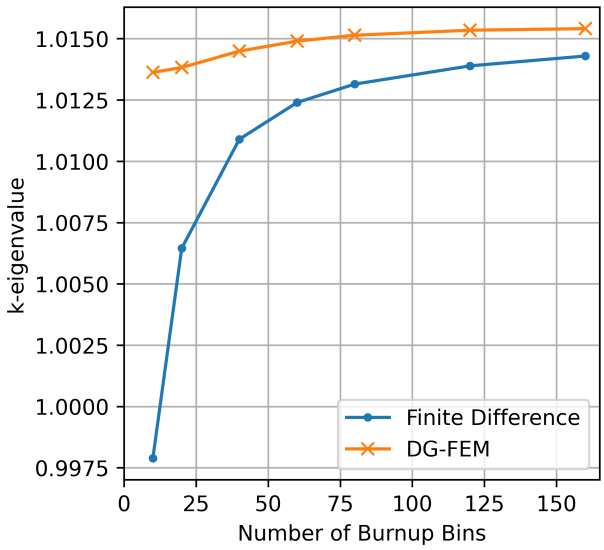

Figure 2. Schematic showing the model used for numerical investigations with the streamlines shown in yellow running through the core region. Also shown is the equilibrium core power density for the model.

final burnup bin is infinite in size. Pebbles can flow into it, but not out of it as it has no upper bound.

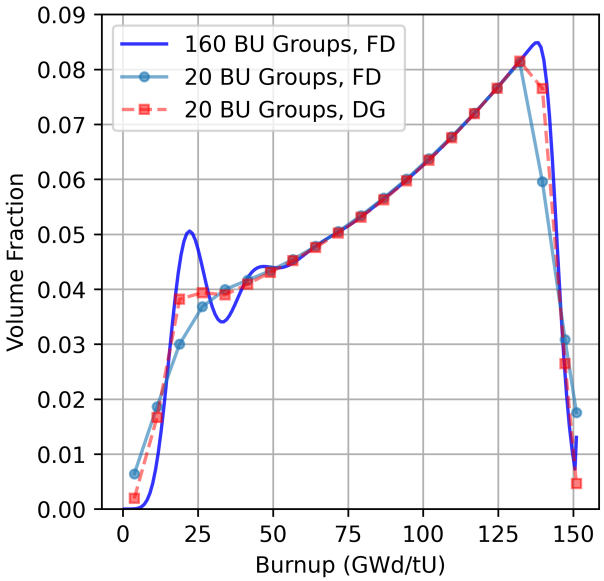

Figure 3. Schematic showing the model used for numerical investigations with the streamlines shown in yellow running through the core region. Also shown is the equilibrium core power density for the model.

It is apparent when comparing the 160 bin FD discretization result to the 20 bin result that the FD discretization is unable to produce the same fine level of detail. The important aspect of this, which is related

to the eigenvalue calculation, is that the lower resolution result over predicts the amount of pebbles with low burnup and as a result of this, under predicts the amount of pebbles past the burnup limit that need to be discarded and replaced with fresh fuel.

Figure 3 also shows a result using DG-FEM. In this case, the predicted k-eigenvalue with only 20 burnup bins is already 1.0138 which is only tens of pcm different from the highly refined FD discretization result. Figure 3 shows that the DG-FEM discretization is better able to capture the peak in volume fraction from the single pass pebbles and therefore predicts more pebbles with burnup past the limit. Figure 2 also shows a convergence study result for DG-FEM. It is noted that more grid study was performed than is included in this plot. From 500 to 750 burnup bins, the FD method predicts the k-eigenvalue increase from 1.015073 to 1.015197 while for DG-FEM, the k-eigenvalue increases from 1.015344 to 1.015408 going from only 120 burnup bins to 160 bins. Thus FD is very slowly converging relative to DG-FEM. The two methods are converging to nearly the same k-eigenvalue, however, it's not clear they should converge to the exact same value since a conservative fixup is being used with the DG-FEM method to avoid negative densities and volume fractions during the calculation.

3. CONCLUSIONS

Verification efforts of the streamline PBR depletion capability in Griffin have included basic numerical studies as well as code-to-code benchmarks. This work documented specific numerical studies into burnup space discretization, which is of particular interest because of the unique way Griffin computes pebble burnup. The simple FD numerical method initially implemented in Griffin was found to have a significant drawback specifically related to k-eigenvalue results for PBR simulations with pebble recycling. It was found that the k-eigenvalue results are sensitive to accurately predicting the volume fraction of pebbles that have gone beyond the burnup limit. The newly implemented DG numerical method was able to much more quickly converge to the correct burnup space distribution which was shown in this work to be a relatively complex shape.

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