Explicit Modeling of Pebble Temperature in the Porous-medium Framework for Pebble-bed Reactors Applications

Nuclear Science and Engineering Division

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ABSTRACT

In this study, an explicit model for pebble temperature calculations in the framework of a porous-medium approach has been developed and implemented in the SAM code. The solid-phase energy conservation equation, including the explicit modeling of pebble temperature, is a multi-scale model, which can predict the macroscopic (pebble-bed) and microscopic (pebble) temperature distributions under both steady-state and transient conditions. Extensive and successful code verifications and demonstrations have been performed for this newly developed model. By explicitly modeling pebble temperatures, this new model addresses a major deficiency of the previously implemented model, which assumed a local solid-phase thermal equilibrium that is not appropriate for pebble-bed reactor design and safety analysis applications.

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1 Introduction

In pebble-bed reactor designs, such as pebble-bed high-temperature gas-cooled reactors (PB-HTGRs) and pebble-bed fluoride salt-cooled high-temperature reactors (PB-FHRs), it is of particular importance to accurately predict pebble temperatures for both normal operating and transient conditions. In most existing designs, fuel pebbles are made of graphite (which also serves as moderator) with TRISO fuel particles dispersed in it. The temperatures of both the graphite matrix and fuel particles are essential to the design and safety analysis of pebble-bed reactors. Under normal reactor operating conditions, it is important to make sure that fuel kernel temperatures are within design limits. In certain reactor transients, when decay heat must be removed, it is essential to maintain the peaking fuel kernel temperature within safety limits. In other types of transients, such as Anticipated Transient Without Scram, it is critical to predict both graphite (as moderator) and fuel temperatures for accurate estimations of reactivity feedback.

To address modeling and simulation needs of pebble-bed reactor designs, a porous-medium-based multi-dimensional model has been implemented in the SAM code [1][2]. The implemented porous-medium model includes mass, momentum, and energy balance equations for the fluid phase, as well as an energy balance equation for the solid phase. Some issues have been revealed in previous studies indicating that the solid-phase energy equation is not suitable for pebble-bed reactor analysis, because inappropriate assumptions and simplifications are made in the averaging process. In the remainder of this section, the existing porous-medium model and its issues for pebble-bed reactor analysis will be discussed. In Section 2, a new multi-scale explicit model for accurate pebble temperature predictions will be presented. Section 3 discusses code implementation within the MOOSE's finite element method (FEM) framework. Section 4 and 5 provide extensive code verifications and code demonstrations in a reference PB-FHR design, respectively. Conclusions and discussion of future work are presented in Section 6.

1.1 Existing Model

As discussed by Nield and Bejan [3], in porous media, the laws that govern the macroscopic variables can be obtained by averaging the standard (microscopic) equations obeyed by the fluid and solid phases. The two commonly used averaging processes are spatial averaging over a sufficiently large representative elementary volume (r.e.v.) and ensemble (statistical) averaging over many, ideally an infinite number of, realizations. Both averaging processes are also fundamental to the theory of two-phase flow [4]. Although spatial averaging is more straightforward and intuitive, ensemble averaging offers subtle advantages that lead to mathematically more rigorous theories. For the applications we are interested in, the two approaches are essentially the same, although the ensemble average might be able to overcome some difficulties associated with the derivation of the pebble-bed effective heat conduction term, as discussed later in Section 2. We followed the porous-medium models described by Nield and Bejan [3] and introduced necessary extensions to bridge the convective heat transfer between the two phases, and to include the pebble-bed-scale heat conduction. The macroscopic model, or the porous-medium model, consists of a set of balance equations for the fluid phase and an energy balance equation for the solid phase, which are summarized as follows:

$$\epsilon \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (1)$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \frac{\rho}{\epsilon} (\mathbf{v} \cdot \nabla) \mathbf{v} + \epsilon \nabla p - \epsilon \rho \mathbf{g} + \beta \mathbf{v} + \alpha |\mathbf{v}| \mathbf{v} = 0, \quad (2)$$

$$\epsilon \rho c_p \frac{\partial T}{\partial t} + \rho c_p \mathbf{v} \cdot \nabla T - \nabla \cdot (\epsilon k \nabla T) - q''' + a_w h(T - T_s) = 0, \quad (3)$$

$$(1 - \epsilon) \rho_s c_{p,s} \frac{\partial T_s}{\partial t} - \nabla \cdot (k_{s,eff} \nabla T_s) - q_s''' + a_w h(T_s - T) = 0, \quad (4)$$

where subscript s denotes the solid phase, ϵ is the porosity of the pebble bed, and $\mathbf{v}$ is the so-called superficial velocity, which is related to the intrinsic velocity $\mathbf{V}$ by $\mathbf{v} = \epsilon \mathbf{V}$. More details of this set of equations are given in references [1] and [2]. The model is similar to the model used in other computer codes, such as Pronghorn [5][6]. Hereafter, we shall refer to this model as the “standard model.”

1.2 Issue with the Current Solid Energy Equation

The issue with the solid-phase energy equation (4) of the standard model is that it is only valid when a local solid-phase thermal equilibrium is assumed. This means that the solid particles in the porous medium have to be thermally thin, such that the temperature gradient within them is sufficiently small to be ignored. This is, unfortunately, not true for pebble-bed reactors. The issue can be more clearly explained by examining the definitions of the various solid temperatures in the different terms of the solid-phase energy equation. Without the need to formally define these averaged temperatures, it is still easy to see that the averaged solid temperature T_s in the transient term, i.e., $(1 - \epsilon) \rho_s c_{p,s} \frac{\partial T_s}{\partial t}$, is associated with the volume average of particle temperatures in the r.e.v.; while T_s in the last convective heat transfer term, i.e., $a_w h(T_s - T)$, is clearly associated with the particle surface area average of solid temperature, because the fluid phase only “sees” the surfaces of particles. Clearly, these two averaged temperatures are not necessarily the same, and in general, they are not the same for pebble-bed reactors because of heat generation internal to the fuel pebbles. Lastly, the second term of the equation, i.e., the diffusion term, represents a collective effect of multiple heat-transfer mechanisms in a pebble bed, such as heat conduction in solid particles, contact heat conduction between solid particles, heat conduction in the fluid phase, and solid-to-solid thermal radiation heat transfer [7]. It is indeed a challenging task to appropriately define the averaged solid temperature for this term, given the complex heat transfer mechanisms involved, and to the authors’ best knowledge, this solid temperature has never been appropriately defined.

To further illustrate the issue with the current solid-phase energy equation, it can be put in the context of safety analysis of pebble-bed reactors. For a scenario where a transient is initiated after the reactor reaches a steady state, with the solid-phase energy equation (4), the predicted steady-state pebble temperature is essentially the surface temperature. However, in reality, the pebble’s interior temperature is higher than its surface temperature because of fission power generated internally in each pebble. This means an underestimated stored thermal energy prediction of the pebble bed for the following transient analysis to start with, which, in consequence, represents a non-conservative assumption for reactor safety analysis.

2 Explicit Modeling of Pebble Temperature

To address the modeling deficiency issue discussed in the previous section, the solid-phase energy equation (4) has to be reformulated. One possible way is to reformulate the original equation (4) by appropriately performing an averaging process on the microscopic solid heat conduction equation over the r.e.v. The shortcoming of this approach is that there will appear multiple averaged solid temperatures in the solid-phase energy equation, as sketched in the previous section, and additional assumptions/approximations must be provided to close the equation system. As discussed in the previous section, at least two averaged solid-phase temperatures, i.e., volume-averaged and surface-averaged ones, will appear. Additional approximations, such as quasi-steady-state condition, have to be introduced to link the two averaged temperatures, in order to appropriately close the equation system. Such an approximation will work well for steady-state solutions; however, it is not suitable for transient simulations.

In this work, we propose a new multi-scale approach that extends the original porous-medium model solid-phase energy equation to include an explicit modeling of pebble temperature in one-dimensional spherical coordinates. Figure 1 shows the concept of an r.e.v. in the context of pebble beds. As discussed by Nield and Bejan [3], the length scale of such a volume must be much larger than the pore/particle scale, but considerably smaller than the length scale of the macroscopic flow domain. In pebble-bed reactor applications, we assume that such a volume encloses a number of pebbles, which, on average, behave similarly from the thermal fluid perspective. Because of significant fission/decay power released internally in pebbles, we no longer assume that they are in local thermal equilibrium. Within the r.e.v., we will assume the following:

- 1) The heat generation is uniformly distributed among all pebbles, a reasonable assumption given that the length scale of an r.e.v. is much smaller than the reactor scale; and
- 2) For the fluid phase, the flow quantities of interest are only of concern in an averaged manner, which is reasonable and practical, given that the pore length scale is much smaller than the r.e.v. length scale and the detailed pore-scale flow behavior is of no particular interest.

Figure 1: The concept of a representative elementary volume (r.e.v.) illustrated in the pebble-bed condition: the r.e.v. is represented by a dashed circle at the left, and an enlarged representative pebble in the r.e.v. is shown at the right.

With these two assumptions, all the pebbles in the r.e.v. can be represented by a “representative pebble,” as shown in Figure 1, whose temperature can be modeled by a one-dimensional heat conduction equation in a local spherical coordinate,

$$\rho_s c_{p,s} \frac{\partial T_p}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T_p}{\partial r} \right) + q''' \quad \text{for } 0 \leq r \leq R, \quad (5)$$

in which the subscript ‘ p ’ denotes pebble and R is the radius of pebbles. It is noted that equation (5) has not been appropriately closed, since the boundary condition on the pebble surface is still missing, as discussed below.

We will develop the pebble surface temperature model using a two-step approach. In the first step, on pebble surfaces, it is assumed that there is no heat exchange between pebbles, and the only heat transfer mechanism is pebble-to-fluid convective heat transfer. As shown in Figure 2, pebbles are artificially moved away from each other to emphasize the absence of pebble-to-pebble heat transfer. Considering energy balance for a thin layer of infinitesimal thickness across the pebble surface,

$$4\pi R^2 \delta \frac{dT_{ps}}{dt} = 4\pi (R^-)^2 \left(-k_s \frac{\partial T_p}{\partial r} \Big|_{ps} \right) - 4\pi (R^+)^2 h (T_{ps} - T_f), \quad (6)$$

in which δ is the thickness of the thin layer, $R^- = R - \delta/2$ and $R^+ = R + \delta/2$. The subscript ‘ ps ’ denotes pebble surface. As δ tends to zero, the first term of equation (6) tends to zero, and the energy balance can be simply stated as

$$-k_s \frac{\partial T_p}{\partial r} \Big|_{ps} = h (T_{ps} - T_f). \quad (7)$$

If the pebble-to-pebble heat transfer is not considered further, the solid-phase energy equation (4) can be replaced with the explicit pebble heat conduction equation (5) in combination with the pebble surface energy balance equation (7), which properly bridges the solid- and fluid-phase temperatures, i.e., the equations are already appropriately closed.

Figure 2: Energy balance for the thin layer across the pebble surface with infinitesimal thickness, assuming there is no pebble-to-pebble heat transfer.

The next step is to include the pebble-to-pebble heat transfer. This process is illustrated in Figure 3. For the infinitesimal layer, besides the conduction heat flux and pebble-to-fluid convective heat fluxes, heat is also transferred from a pebble to its surrounding pebbles via solid-contact heat conduction, fluid-phase heat conduction, and solid-to-solid thermal radiation heat transfer [7]. This pebble-to-pebble heat flux is denoted as q''_{p-p} , in which the subscript “ p - p ” means pebble-to-pebble. This heat-flux term only represents a collective effect and therefore it represents a pebble surface averaged value. Similar to equation (7), the new energy balance equation can be obtained for this thin layer:

$$q''_c = q''_{conv} + q''_{p-p}$$

with $q''_c = -k_s \frac{\partial T_p}{\partial r} \Big|_{ps}$ and $q''_{conv} = h(T_{ps} - T_f)$ (8)

Figure 3: Energy balance for the thin layer across the pebble surface with infinitesimal thickness, considering pebble-to-pebble heat transfer.

However, additional manipulation is needed to connect the q''_{p-p} term in equation (8) to the pebble-bed effective heat conduction term $\nabla \cdot (k_{s,eff} \nabla T_s)$ in equation (4). To do so, various concepts associated with pebble-bed r.e.v. will be introduced and defined. As shown in Figure 4, we denote the r.e.v. as V , and the pebble surfaces that are enclosed in volume V are denoted as A_i (the red lines). The surface of volume V , denoted as ∂V , intersects with several pebbles (the shaded ones) partially enclosed in the volume. The intersected surface is denoted by ∂V_I (not illustrated).

Figure 4: Various concepts associated with pebble-bed representative elementary volume.

We then perform a surface integral of equation (8) over the interface A_i to obtain

$$\int_{A_i} \mathbf{q}_c'' \cdot \hat{\mathbf{n}} dA = \int_{A_i} \mathbf{q}_{conv}'' \cdot \hat{\mathbf{n}} dA + \int_{A_i} \mathbf{q}_{p-p}'' \cdot \hat{\mathbf{n}} dA, \quad (9)$$

in which $\hat{\mathbf{n}}$ is the out norm. We now define the averaged pebble surface area per unit elementary volume, which is also known as the heating surface area density, as

$$a_w = \frac{A_i}{V} \quad (10)$$

With this definition, equation (9) can be written as

$$\int_V q_c'' a_w dV = \int_V q_{conv}'' a_w dV + \int_{A_i} \mathbf{q}_{p-p}'' \cdot \hat{\mathbf{n}} dA \quad (11)$$

Note that, since q_{p-p}'' is already an averaged value for each pebble and is constant for them, for the last term of equation (11), the surface integral on the surface of any pebble completely enclosed within the elementary volume is zero. The remaining non-zero part can be rewritten as

$$\begin{aligned} \int_{A_i} \mathbf{q}_{p-p}'' \cdot \hat{\mathbf{n}} dA &= \int_{\partial V_I} -\mathbf{q}_{p-p}'' \cdot \hat{\mathbf{n}} d(\partial V_I), \\ &= \int_{\partial V} -\mathbf{q}_{p-p}'' \cdot \hat{\mathbf{n}} (1 - \epsilon) d(\partial V), \\ &= - \int_V \nabla \cdot (\mathbf{q}_{p-p}'' (1 - \epsilon)) dV, \end{aligned} \quad (12)$$

in which the first equal sign is obtained by applying the Divergence Theorem, the second equal sign assumes that surface porosity is the same as volume porosity, and the last equal sign is obtained by applying the Divergence Theorem to the elementary volume. With equation (12), equation (11) can be rewritten as

$$\int_V q_c'' a_w dV = \int_V q_{conv}'' a_w dV - \int_V \nabla \cdot (\mathbf{q}_{p-p}'' (1 - \epsilon)) dV \quad (13)$$

or, without the volume integral (since the volume is arbitrary),

$$a_w q_c'' = a_w q_{conv}'' - \nabla \cdot (\mathbf{q}_{p-p}'' (1 - \epsilon)) \quad (14)$$

At this stage, it does not seem that equation (14) could be further manipulated, and we have to *deduce* that the last pebble-to-pebble heat transfer term is indeed the pebble-bed effective heat conduction term¹, and therefore, equation (14) is rewritten as

$$-a_w q_c'' + a_w h(T_{ps} - T_f) - \nabla \cdot (k_{eff} \nabla T_{ps}) = 0 \quad (15)$$

Note that the original T_s in the diffusion term has been replaced with T_{ps} in equation (15) for pebble surface energy balance.

To summarize, in the newly proposed multi-scale modeling approach, the original single solid energy equation

$$(1 - \epsilon) \rho_s c_{p,s} \frac{\partial T_s}{\partial t} - \nabla \cdot (k_{s,eff} \nabla T_s) - q_s''' + a_w h(T_s - T) = 0 \quad (4)$$

is replaced with the modified porous-medium model equation, or the pebble surface energy balance equation,

$$-a_w q_c'' + a_w h(T_{ps} - T_f) - \nabla \cdot (k_{eff} \nabla T_{ps}) = 0, \quad (15)$$

and an additional pebble heat conduction equation,

$$\rho_s c_{p,s} \frac{\partial T_p}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T_p}{\partial r} \right) + q_s''' \quad (5)$$

The pebble surface energy balance equation connects the pebble internal heat conduction to the pebble-to-fluid convective heat transfer and the pebble-bed effective heat conduction. Hereafter, we shall refer to this model as the “explicit pebble model.”

¹ One can find the similarity between the term $\nabla \cdot (\mathbf{q}_{p-p}'' (1 - \epsilon))$ and the term $(1 - \epsilon) \nabla \cdot (k_s \nabla T_s)$ of equation (2.1) from Nield and Bejan [3]. In addition, as explained in [2], the pebble-bed effective heat conduction term $\nabla \cdot (k_{s,eff} \nabla T_s)$ is merely a replacement term for $(1 - \epsilon) \nabla \cdot (k_s \nabla T_s)$.

3 Code Implementation

SAM is a computer code based on the MOOSE framework [8], which provides a FEM for spatial discretization of partial differential equations and various types of time integration schemes. The resulting discretized non-linear equation system is solved with the Jacobian-free Newton-Krylov method provided by PETSc [9] through the MOOSE framework interface. In a previous report [2], details of the code implementation of SAM’s porous-medium model have been discussed, including the FEM weak forms of porous-medium model equations and necessary stabilization schemes.

In this report, we will be focused on the code implementation of the reformulated solid-phase energy equations, i.e., both the pebble surface energy balance equation and the explicit pebble heat conduction equation. Similar to the original solid energy equation and other porous-medium flow equations, the pebble surface energy balance equation “lives” on the global pebble-bed coordinates, and its FEM formulation and code implementation are similar to those equations. The pebble heat conduction equation, however, needs special treatment, since it uses *local* spherical coordinates. The most intuitive way to deal with this localized equation is to directly use MOOSE’s mesh and FEM support. However, there are several difficulties/inconveniences associated with this approach. First, two sets of meshes will be needed, one for the global mesh (i.e., the pebble bed), and another one for pebbles (consisting of many pieces of local meshes). Depending on the resolution needed for local pebbles to be modeled, it could be a requirement to have a pebble mesh per node, element, or sub-block of the global mesh. Second, the local pebble mesh setup requires additional manual/automatic generation of meshes besides the global mesh; and the local pebble heat conduction equation requires additional input files to set up the problem. Third, the coupling between the global mesh physics (porous-medium model) and the local mesh physics (pebble heat conduction) requires MOOSE’s MultiApp execution, which requires Picard iterations for the simulation to converge and adds additional computational cost.

Figure 5: Problem and mesh setup for the hybrid finite-element/finite-volume method.

To address these potential issues, we propose to use a hybrid finite-element/finite-volume method approach. The local pebble heat conduction equation per element of global mesh is handled with the finite-volume method. The hybrid approach is illustrated in Figure 5. The variables associated with the macroscopic porous-medium model, including fluid pressure p , velocity $\mathbf{v}$, temperature T_f , and pebble surface temperature T_{ps} , are arranged on the global mesh

as nodal variables, e.g., first-order Lagrange variables. The pebble temperature, T_p , is defined for each element of the global mesh as MOOSE's ArrayVariable, e.g., constant monomial variable with component N representing total number of layers (finite volumes) to discretize pebble temperature in the radius direction, shown in Figure 5.

The finite volume discretization scheme is quite standard, and only some brief discussion is provided. The local mesh setup is shown in Figure 6. For the i -th finite volume, the discretized equation is

$$V_i \rho_{s,i} c_{p,s,i} \frac{dT_{p,i}}{dt} = q''_{i-1/2} A_{i-1/2} - q''_{i+1/2} A_{i+1/2} + V_i q''' , \quad (16)$$

in which

$$q''_{i-1/2} = k_{s,i-1/2} \frac{T_{p,i-1} - T_{p,i}}{\Delta r}$$

$$A_{i-1/2} = 4\pi r_{i-1/2}^2$$

$$V_i = \frac{4}{3}\pi(r_{i+1/2}^3 - r_{i-1/2}^3)$$

$$\Delta r = r_{i+1/2} - r_{i-1/2}$$

For the pebble surface, the heat conduction heat flux, i.e., q''_c of equation (15), is approximated as

$$q''_c = k_{s,N} \frac{T_{p,N} - T_{ps}}{\Delta r/2} ,$$

in which $T_{p,N}$ is the pebble temperature of the N -th finite volume, and T_{ps} is the coupled pebble surface temperature that is defined on the global mesh. Note that the same q''_c appears in both the pebble heat conduction equation for the N -th finite volume and the pebble surface energy balance equation, and thus links the local pebble heat conduction equation with the macroscopic porous-medium models. The time-dependent term, $dT_{p,i}/dt$, is left for MOOSE to handle, depending on the specific time integration scheme users specify, e.g., BDF2 as the default scheme.

Figure 6: Finite-volume method to discretize the one-dimensional pebble heat conduction equation.

4 Code Verification

In this section, multiple verification tests are included for code verification of the newly implemented multi-scale solid energy equation. These steady-state and transient test cases are designed to verify the various terms of the model, such as the spatial discretization of the heat conduction term, the time integration scheme (directly using MOOSE-provided implementation) of the transient term of the explicit pebble temperature model, the convective heat transfer term in both the macroscopic solid energy equation and fluid-phase energy equation, and the effective thermal conduction term in the macroscopic solid energy equation. These verification test cases are discussed in the subsections that follow.

4.1 Heat Conduction Verification Test

In this verification test, the spatial discretization of the finite volume method is verified. The test case is a simple spherical heat-conduction problem with a constant pebble surface temperature T_{ps} and a constant volumetric heat source q''' . The analytical solution for equation (5) in the steady state can be easily obtained as

$$T(r) = T_{ps} + \frac{q'''}{6k_s}(R^2 - r^2) \quad (17)$$

For this verification test, the following values are used: $q''' = 1.9 \times 10^7 \text{ W/m}^3$, $R = 0.06 \text{ m}$, $k_s = 30 \text{ W/m-K}$, and $T_{ps} = 100 \text{ K}$, as shown in Figure 7.

Figure 7: Problem setup for the pebble heat conduction verification test.

SAM simulations are performed in a 1-m by 1-m (x by y) square domain using 5 by 5 uniform mesh. The pebble surface temperature T_{ps} is modeled as a MOOSE AuxVariable, which has been set at a constant value of 100 K. In each element, transient pebble temperatures are solved from the discretized pebble heat conduction equation, and steady-state solutions are obtained at the end of the transient simulations. Numerical simulations are performed using different numbers of finite volumes (layers) for pebbles. As shown in Figure 8 (left), steady-state pebble temperature solutions using 5 and 10 finite volumes per pebble are compared with the analytical solution, equation (17). Both numerical results show good agreement with analytical solutions; for $N = 5$, the averaged error between numerical results and analytical solutions is 3.8 K, and for $N = 10$, the averaged error is 0.95 K.

Additional verification is performed by means of a mesh refinement study. For the same problem, pebble mesh numbers were refined from 5 to 10, 20, and 40, to study the L2 norm of numerical error, which follows the definition given by LeVeque [10] and is defined as

$$\|E\|_2 = \sqrt{\Delta r \sum_{i=1}^N (u_{num} - u_{ana})^2} \quad (18)$$

Figure 8 (right) plots the L2 error norm against the number of finite volumes. In a log-log plot, it follows exactly a straight line with a slope of -2, which verifies that the implemented finite volume method provides a second-order spatial accuracy, as expected.

Figure 8: Comparisons between SAM-predicted numerical results: (left) dots, using 5 and 10 finite volumes, and analytical solution, shown by solid line; (right) second-order spatial accuracy of the implemented finite volume method.

4.2 Convective Heat Transfer Verification Test

In this verification test, the main focus is to verify the spatial discretization of the finite volume method, the time integration scheme, and the convective heat transfer boundary condition of pebbles. As illustrated in Figure 9, the test case is a transient “quenching” problem, with the pebble at an initial temperature T_0 submerged in a fluid with a constant temperature T_f . There is no internal heat source for the pebbles, so the pebble temperature decreases with time via convective heat transfer to the fluid phase. The analytical solution to the transient problem is given by Taler and Oćłoń [11]:

$$\vartheta(\eta) = \sum_{n=1}^{\infty} \frac{2(\sin\mu_n - \mu_n \cos\mu_n)}{\mu_n - \sin\mu_n \cos\mu_n} \frac{\sin(\mu_n \eta)}{\mu_n \eta} e^{-\alpha w_n^2 t}, \quad (19)$$

in which α is the thermal diffusivity and t is time. The nondimensional radius and temperature are

$$\eta = r/R$$

$$\vartheta(\eta) = \frac{T_p(R\eta, t) - T_f}{T_0 - T_f} = \frac{T_p(r, t) - T_f}{T_0 - T_f}$$

The values of μ_n can be found as the roots of the characteristic equation:

$$\tan(\mu) = \frac{\mu}{1 - \text{Bi}} , \quad (20)$$

in which Bi is the Biot number, and $\text{Bi} = hR/k_s$. w_n is defined as

$$w_n = \mu_n/R$$

Figure 9: Problem setup for the pebble convective heat transfer verification test.

For this verification test problem, we have set $T_0 = 200$ K, $T_f = 100$ K, $\alpha = 10^{-5}$ m²/s, $k_s = 40$ W/m-K, $R = 0.02$ m, and $h = 4 \times 10^3$ W/m²-K, which correspond to $\text{Bi} = 2.0$. Similarly to the simulation discussed in the previous heat conduction verification test, SAM simulations are performed in a 1-m by 1-m (x by y) square domain using 5 by 5 uniform mesh. The fluid temperature T_f is modeled as a MOOSE AuxVariable, which has been set at a constant value of 100 K. The pebble surface temperature T_{ps} is solved from the pebble surface energy balance equation (15). For this problem, the pebble-bed effective heat conduction term $\nabla \cdot (k_{s,eff} \nabla T_s)$ is excluded by setting $k_{s,eff} = 0$.

Figure 10 shows the comparison between SAM-predicted transient numerical results (dots) and analytical solutions (solid lines) at different times, using 10 and 20 finite volumes per pebble and $\text{Bi} = 2.0$. Very good agreements between simulations and analytical solutions are found from the plots. For example, at time = 20 s, the averaged error is 0.084 K for $N = 10$, and 0.023 K for $N = 20$.

An additional case is included in this verification test with $\text{Bi} = 1.0$ and $h = 2 \times 10^3$ W/m²-K; all other parameters are kept the same. The results (Figure 11) show good agreement between numerical results and analytical solutions.

Bi = 2

Figure 10: Comparisons between SAM-predicted numerical results (dots) and analytical solutions (solid lines) for the convective heat transfer verification problem at time $t = 5, 10$, and 20 s, for $N = 10$ (left) and $N = 20$ (right), with $Bi = 2$.

Bi = 1

Figure 11: Comparisons between SAM-predicted numerical results (dots) and analytical solutions (solid lines) for the convective heat transfer verification problem at time $t = 5, 10$, and 20 s, for $N = 10$ (left) and $N = 20$ (right), with $Bi = 1$.

4.3 Energy Balance Verification

In this verification test, the main focus is to verify the energy balance between heat generation in pebbles and enthalpy increase in the fluid phase of a porous medium. The problem of this energy balance test case is set up in a rectangular two-dimensional porous medium, 1 m (x) by 0.1 m (y), as shown in Figure 12. For the fluid phase, the inlet conditions are given at the left boundary with inlet temperature T_{in} and velocity v_{in} , and an outlet pressure p_{out} is given at

the right outlet boundary. The top and bottom boundaries are set as non-penetrating and slip boundaries. For the solid phase, the pebble has a radius of 0.03 m and a uniformly distributed constant volumetric heat source of 10^6 W/m³. The porosity of the pebble bed is set to be 0.6. For this problem, the pebble-bed effective heat conduction term $\nabla \cdot (k_{s,eff} \nabla T_s)$ is excluded by setting $k_{s,eff} = 0$.

Figure 12: Problem setup for the energy balance verification test.

As convective heat transfer between the fluid phase and pebbles is the only heat transfer mechanism, the fluid-phase temperature is expected to increase linearly in the x-direction, assuming that the fluid has a constant specific heat capacity. The analytical solution for the fluid-phase temperature can be expressed as

$$T_f(x) = T_{in} + \frac{\epsilon q''' x}{\rho_{in} v_{in} c_p}, \quad (21)$$

in which $\rho_{in} = 77$ kg/m³ is the fluid density at the inlet; $v_{in} = 1$ m/s is the inlet velocity; $T_{in} = 630$ K is the inlet temperature; and $c_p = 100$ J/kg-K is the specific heat capacity.

Two-dimensional SAM simulations were performed using a 20 by 8 (x by y) uniform mesh, using both the new multi-scale solid-phase energy equations (the explicit pebble model) and the original single-equation model (the standard model). Null transient simulations were performed for both cases, and steady-state solutions were obtained at the end of the simulations. SAM-predicted numerical results are plotted with analytical solutions in Figure 13. For both models, at the steady state, SAM-predicted fluid temperatures are well overlapped with the analytical solution, which demonstrates a successful verification of the energy balance between the pebble heat generation and fluid-phase heat-up.

More importantly, the standard model treats the solid phase as one in local thermal equilibrium, and therefore, it only models a single solid temperature, T_s (Figure 13, right). On the contrary, the new model includes an explicit model for pebble temperature, so it models not only the pebble surface temperature, T_{ps} , but also the radially distributed pebble temperature. In the left plot of Figure 13, for the radially distributed pebble temperature, only the pebble center temperature is shown. It is noted that, since pebble temperatures are defined as constant in each element, the pebble center temperature is shown as a step function of x . From the two plots of Figure 13, it is also clear that the solid temperature predicted using the standard model is merely the pebble surface temperature predicted with the new model, which is a model issue highlighted in Section 1.2.

Figure 13: Comparison between SAM-predicted results and analytical solution, using both the new model and the original model for the solid-phase energy equation.

4.4 Pebble-bed Effective Heat Conduction Verification

The main purpose of this verification test is to verify that the reformulated solid-phase energy equation is still able to correctly model the pebble-bed effective heat conduction and predict the correct macroscopic pebble-bed solid temperatures. For this verification test, we reuse one of the test cases from a previous code validation study [1], i.e., the High Temperature Test Unit (HTTU) test case. The HTTU facility, developed by the PBMR company in collaboration with North-West University and M-Tech Industrial (Pty) Ltd. in South Africa, is an experiment facility dedicated to studying the different thermal-fluid phenomena of the PB-HTGR [12]. A separate effect test has been performed to investigate the effective thermal conductivity of the pebble bed.

Figure 14 shows a schematic drawing of the HTTU test facility, which consists of approximately 25,000 graphite pebbles randomly packed within an annular core configuration bounded by inner and outer graphite reflectors. The facility was filled with nitrogen gas at 0.1 atm to reduce heat transfer due to gas natural convection. A set of heater elements/electrodes were inserted in the inner graphite reflector region to provide heat to the pebble bed, while the outer reflector was enclosed within a water-cooled jacket, which removes the heat. The top and bottom of the pebble bed were thermally well-insulated to limit heat loss.

Figure 14: Vertical cut through the HTTU test section.

Figure 15 shows the problem setup of the HTTU test case for the SAM input model using a two-dimensional RZ geometry. Uniform-sized meshes are used for both the reflector block (5×10 , $R \times Z$) and the pebble-bed block (40×10 , $R \times Z$). In the reflector block, the heat conduction equation was solved, and in the pebble bed, the solid-energy equations include the pebble heat conduction equation and the pebble surface energy equation. Similarly to the test cases used in the previous validation study [1], both the 82-kW and 20-kW test cases are studied, and the boundary conditions are listed in

Table 1.

Figure 15: Problem setup of the HTTU test case.

Table 1: Input parameters for SAM HTTU validation

	82-kW Case	20-kW Case
Heat rate [kW]	66.27	11.92
q''_{BC} [W/m ²]	43946.66	7904.70
T_{BC} [°C]	104.57	46.67

Using the explicit pebble model, transient SAM simulations were performed to obtain pebble-bed solid temperatures. Steady-state solutions were obtained at the end of the transient simulations. Figure 16 shows the pebble temperatures predicted using the new model, including both the pebble surface and center temperatures, for both the 82-kW and 20-kW cases. Figure 16 shows that, in the steady state, the pebble center temperature (plotted as step functions) matches the locally averaged pebble surface temperature, which is expected, as there is no internal heat source. Figure 16 also shows that the pebble surface temperatures from the new model overlap well with the results predicted with the previous standard model [1]. This overlap verifies that the new model is able to correctly model the pebble-bed effective heat conduction macroscopic behavior.

Figure 16: Comparisons of pebble surface temperatures between the new explicit pebble model T_{ps} and the standard model T_{ps} (reference) [1].

5 PB-FHR Code Demonstration

In this section, the updated porous-medium model will be demonstrated using a more realistic and complex reference PB-FHR model developed from a previous study [13]. The generic PB-FHR model was based on the University of California, Berkeley, Mk1 design [14], but incorporated some design characteristics of a preliminary commercial FHR design because of its higher readiness for licensing application. The primary system of the generic PB-FHR model is shown in Figure 17, which is based on the Mk1 SAM model presented in reference [13]. Upon exiting the salt collection ring within the graphite reflector, the hot salt travels upwards, 1, where it exits the reactor vessel. The hot salt then passes the expansion tank, 2, and enters the primary coolant pump, 3. After exiting the pump, the hot salt passes through a helical heat exchanger, 4, where energy is transferred to “solar” salt, 7. The cooled salt then passes through a network of piping, 5, until it reaches the reactor vessel and is distributed within the downcomer, 6. The pipes that compose the primary system are assumed to be 24-in. Schedule 80 pipe. To prevent the primary salt velocity from exceeding 2 m/s, an identical second primary loop is introduced.

Two demonstration cases are presented in this section. In the first case, for the purpose of simplicity, a standalone two-dimensional PB-FHR core model is used. The goal is to demonstrate that the new model works well in a complex core model that includes both a porous-medium model for the pebble bed and a heat-conduction model for reflectors, as well as the heat transfer between the pebble bed (porous-medium) and adjacent solid structures (heat conduction). In the second case, the standalone two-dimensional core model is coupled to a one-dimensional system model of the remaining primary system to allow for a system-level simulation.

Figure 17: Graphical representation of the PB-FHR primary system [13].

5.1 Standalone Two-dimensional FHR Core Model

In this demonstration case, the two-dimensional model from the previous study is reused, with only the boundary conditions and reactor power changed to simulate a reactor transient. The two-dimensional RZ model was developed to take advantage of the symmetric feature of

the reactor core, as shown in Figure 18. The 2D mesh contains various blocks and boundaries that allow SAM to apply the appropriate physics in each location. Blocks 11, 12, 13 and 15 are porous zones, which contain a mixture of a coolant and a solid. This arrangement allows the fuel pebbles or porous graphite to be modeled alongside the primary salt. Blocks 11 and 13 correspond to the fueling chute and contraction zone, respectively. Block 12 corresponds to the active fuel region and block 15 corresponds to the salt collection ring. Blocks 2, 3, 4 and 14 are solid zones, where only a solid is defined. The defueling chute, block 14; outer reflector, blocks 4, 5, and 6; and upper reflector, blocks 2 and 3, are modeled as a solid zone because of limited information on the flow paths within each zone.

Figure 18: 2D PB-FHR mesh with blocks (left) and boundaries (right) labeled.

In the previous study, only the steady-state condition was considered for the standalone core model [13]. In this study, to examine how the new multi-scale model improves on the original model, a transient simulation is considered. The simulation is divided into two parts. The first part is from -50000 sec to 250 sec, in which a steady state is reached for the core thermal-fluids condition. At 250 sec, the core inlet velocity starts to decrease to simulate a pump trip scenario, with the normalized inlet velocity given in Figure 19 (left). Meanwhile, the reactor scrams and the core power starts to decrease following a decay heat curve, as shown in Figure 19 (right). During the entire simulation, the core inlet temperature was assumed to be constant.

Figure 19: Normalized inlet velocity (left) and reactor power (right).

SAM transient simulations were performed using both the standard model and the new explicit pebble model in the porous-medium zones (blocks 11, 12, 13 and 15), and the results are plotted in Figure 20. Both models show similar trends in the prediction of core outlet temperature, which decreases first and then increases as a result of the combined effect of decreasing reactor core flow and reactor power. Compared to the results predicted using the standard model, the new explicit pebble model results show a clear increase in the predicted core outlet temperature. This finding verifies that, by including the explicit pebble temperature model, the new model is capable of capturing the extra thermal energy stored in pebbles, which is missed in the original standard model.

Figure 20: Comparison of core outlet salt temperature between the original model and new model.

5.2 Coupled 2D Core and 1D System

In this subsection, the standalone 2D core model presented in the previous subsection is coupled to a 1D system model for the remaining primary system. The coupling is through boundary interface data exchange, as described in reference [13]. The main purpose of this case is to demonstrate that the newly developed model and code implementation work in a very complex input model that requires the use of MOOSE MultiApp and Picard iteration for coupling and MOOSE restart capability for a robust coupling.

Figure 21 shows the problem setup for the coupled 2D core and 1D system input model. The two coupling interfaces are set up at the core inlet and outlet boundaries. For the 2D model, the core inlet and outlet boundary conditions are replaced by the coupling interfaces, where data is transferred from the 1D system model to set up necessary boundary conditions. Additionally, data are transferred back from the 2D core model to the 1D system model on the two coupling interfaces, where the 1D system model boundary conditions are set.

Figure 21: Problem setup for the coupled 2D core and 1D system model.

Similar to the standalone case discussed in the previous subsection, a pump trip accident scenario is modeled. The first part of the simulation covers the interval from -50000 sec to 250 sec, during which a steady state is developed for the primary system thermal-fluids condition. At 250 sec, the primary pump is tripped, and the pump head starts to decrease exponentially as shown in Figure 22. The pump head becomes effectively zero at 290 sec. In this coupled simulation, the primary pump is modeled in the 1D system model, instead of using simplified core inlet velocity boundary conditions as in the previous standalone case. At the same time, the reactor scrams, and the core power is provided as a decay heat curve, the same one used in the standalone case, as shown in Figure 19 (right). The secondary flow of the primary-system heat exchanger has also been reduced to avoid overcooling of the primary-side salt. The time-dependent secondary flow of the heat exchanger is shown in Figure 22 (right).

Figure 22: Normalized primary-pump head (left) and heat-exchanger secondary flow (right).

Coupled simulations for the pump trip accident case were performed using both the original solid-phase energy model and the newly developed multi-scale model for the porous-medium zones. Figure 23 shows the predicted core flow, in terms of core inlet velocity, during the transient. From around 300 to 600 sec, the predicted core flow remains at a relatively stable value, although the pump head has already dropped to effectively zero at around 290 sec. This finding indicates that a natural circulation in the primary system is probably developing. Both models predict very similar values of core flow; however, it can also be observed that the new explicit pebble model result is slightly higher than the value predicted using the original model. Figure 24 shows the predicted core inlet and outlet temperatures. Although the predicted core-inlet velocity and temperature are very similar between the two models, the core-outlet temperature from the new explicit pebble model is about 20 K higher than from the standard model, because the new multi-scale model is able to capture the extra stored thermal energy in pebbles. This factor also explains the finding that the core flow predicted by the new explicit pebble model is slightly higher because of the higher core temperature and the consequently larger buoyancy force.

Figure 23: SAM-predicted core inlet velocities from the original and new models.

Figure 24: SAM-predicted core inlet and outlet temperatures from the original and new models.

6 Conclusions and Future Work

A model deficiency of the solid-phase energy equation in the SAM porous-medium model was reported in the previous applications of pebble-bed reactor thermal-hydraulics analysis. The model deficiency is associated with the assumption of local solid-phase thermal equilibrium, which is not appropriate for pebble-bed reactor applications. To address this issue, a new multi-scale solid-phase energy balance model with explicit modeling of pebble temperature was developed and implemented in SAM within the porous-medium model framework. Compared with the previous model, which assumes local solid-phase thermal equilibrium, the new model employs a one-dimensional transient heat conduction equation in spherical coordinates for pebbles, which can predict a more accurate pebble temperature profile under both steady-state and transient conditions.

For code verification, multiple steady-state and transient test cases were analyzed, with each of them designed to verify the different term(s) of the model, to verify SAM code implementation. This new multi-scale model was then demonstrated in a more complex model for a reference PB-FHR pump trip transient. For the same transient, compared with results from using the previous model, it was clear that the new multi-scale model is able to correctly capture the stored thermal energy in a pebble bed.

Although significant improvement has been made in this work by including an explicit model for pebble temperature in the porous-medium model, additional future studies such as the following can be done to further improve the model fidelity and code usability for pebble-bed reactor simulations:

- Code validation against experimental data with explicit measurements on pebble interior temperatures.
- Inclusion of a fuel-kernel temperature model. The simplest way is to back-calculate fuel kernel temperature from pebble temperature using the explicit model developed in this study, which still only represents locally homogenized graphite/fuel-particle temperature. If higher fidelity is required, an additional model scale for fuel kernels can potentially be added to the multi-scale model.
- Code implementation for the simulations of fuel pebbles with multiple layers of different materials and power densities.

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