Development of a Reference Model for Molten-Salt-Cooled Pebble-Bed Reactor Using SAM

Nuclear Science and Engineering Division

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ABSTRACT

To support the development and utilization of the SAM code for fluoride-salt-cooled high-temperature pebble-bed reactor (PB-FHR) safety analysis and licensing, an effort was devoted to developing reference models for PB-FHR primary loop and the reactor cavity cooling system (RCCS). A reference standard problem of a prototypical reactor design is foundational to NRC to verify the adequacy of computer codes and evaluation models for a specific reactor type.

The SAM code was enhanced for the reference PB-FHR model development, including a 1D-3D flow coupling scheme and conjugate heat transfer between porous media and solid structures. The reference FHR primary loop model was developed based on the UC Berkeley Mk1 FHR design with additional design features from the Kairos Power's KP-FHR core. The PB-FHR core is modeled by a two-dimensional porous medium while the rest of the primary loop is represented by a SAM one-dimensional model. A SAM one-dimensional primary loop model was also developed for comparison using a single channel approach for the reactor core. Furthermore, the water-based NSTF cavity was modeled using SAM multi-dimensional flow module, to assist in evaluating SAM capabilities of modeling the emergency heat removal systems relying on RCCS concepts.

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1 Introduction

An advanced system analysis tool, SAM, is under development for advanced non-LWR reactor safety analysis [1]. It aims to provide fast-running, modest-fidelity, whole-plant transient analyses capabilities, which are essential for fast turnaround design scoping and engineering analyses of advanced reactor concepts. SAM aims to be a generic system-level safety analysis tool for advanced non-LWRs, including Liquid-Metal-cooled fast Reactors (LMR), Molten Salt Reactors (MSR) or Fluoride-salt-cooled High-temperature reactor (FHR), and high-temperature gas-cooled reactor (HTGR). It takes advantage of advances in physical modeling, numerical methods, and software engineering to enhance its user experience and usability.

The molten-salt-cooled pebble-bed reactor, or pebble-bed FHR (PB-FHR) stands out as a promising candidate among advanced nuclear reactor concepts with its improved passive safety characteristics and high thermal efficiency. PB-FHR leverages TRISO fuel in pebble form combined with a low-pressure fluoride salt coolant. Molten fluoride salts have excellent chemical stability and tremendous capacity for transferring heat at high temperature and retaining fission products. The ceramic fuel can maintain structural integrity at extremely high temperatures, which allows significant improvements in cooling capability under accident scenarios.

To support the development and utilization of the SAM code for PB-FHR safety analysis and licensing, a reference primary loop model of PB-FHR is developed using the latest improvements on multi-dimensional flow modeling and 1D-3D coupling techniques in SAM. More specifically, the PB-FHR core is to be modeled by a two-dimensional porous medium model while the external circuits are represented by one-dimensional models for efficient calculation. A reference standard problem of the reactor primary loop model is foundational to the methodologies employed by NRC to verify the adequacy of computer codes and evaluation models. As reactor cavity cooling systems (RCCS) play an important role in the passive safety systems of advanced nuclear reactors, the cavity in a scaled water-based RCCS test facility is modeled and studied in this work to demonstrate SAM's capability in modeling the RCCS.

This report is organized as follows. Section 2 provides a brief description of SAM enhancements for the reference FHR model development, including the 1D-3D flow coupling scheme and the conjugate heat transfer between porous media and solid structures. Section 3 describes the reference FHR model development using SAM and the preliminary simulation results. Section 4 presents the modeling of water-based RCCS cavity with SAM. Lastly, a short summary and follow-up work are discussed in Section 5.

2 Code Enhancements for Reference FHR Model Development

2.1 SAM 3D-1D Flow Coupling Scheme

One of the challenges in predicting dynamical response of pool-type advanced reactors in accident events, such as loss of flow (LOF) accident, is the accurate prediction of multi-scale flow features in reactor components. Three-dimensional flow features inside a large volume, such as the lower and upper plena, can affect the key safety parameters. For example, thermal mixing and stratification in large pools are important phenomena critical to nuclear reactor safety. Modeling and simulation of three-dimensional flow features are mostly limited in the computational fluid dynamics (CFD) analysis of individual component; however, the modeling of these three-dimensional flow components in reactor transient analyses scenario remains a key unresolved, challenging problem. In traditional system analysis codes, simplified zero-dimensional (0-D) or one-dimensional (1-D) models were used to represent these components, which were however not capable of capturing the three-dimensional flow features. In order to perform realistic system analyses, the most straightforward way is to couple the system analysis code to the CFD code.

Recently, SAM was enhanced with capability of modeling a three-dimensional (3-D) flow field [2], which was aimed to reduce the computational resources requirement of typical CFD analysis. However, the current SAM 3-D flow module is not tightly coupled to the SAM 1-D flow module. Because the different scale of computational resource requirements, the 3-D module and 1-D module are solved separately. A multi-scale coupling scheme is needed to couple SAM's 3-D flow module and SAM's 1-D flow module. Unlike the coupling schemes seen in the literatures that require development of additional routine to govern the coupling codes and perform the data transfer between codes, SAM is capable of performing these tasks alone using the MultiApp system of MOOSE.

Figure 2-1. Conceptual scheme of a partitioned non-overlapping 3D-1D flow coupling scheme in SAM

Figure 2-1 shows the schematic of a partitioned non-overlapping 3D-1D flow coupling in SAM. The component (SAM 3-D domain) that involves three-dimensional flow features is partitioned from the main thermal-hydraulics system (SAM 1-D domain). Boundary conditions are exchanged between the 3-D domain and 1-D domain through MultiApp data transfer. Figure 2-2 shows an example of the coupling scheme, where the reactor core is separate from the other

part of the system and modeled with SAM's 3-D module. Data transfer happens in the core inlet and outlet. The exchange of boundary conditions is explained below:

- At the core inlet (location 1):
 - 3-D model: takes the velocity (or mass flux) and temperature transferred from 1-D model as the inlet boundary conditions; record and send to 1-D model the average pressure and temperature at the inlet boundary.
 - 1-D model: takes the pressure and temperature transferred from 3-D model as the outlet boundary conditions (e.g. a time-dependent volume); record and send to 3-D model the outlet velocity and temperature.
- At the core outlet (location 2):
 - 3-D model: takes the pressure transferred from 1-D model as the outlet boundary conditions; record and send to 1-D model the average velocity and temperature at the outlet boundary.
 - 1-D model: takes the velocity and temperature transferred from the 3-D model as the inlet boundary conditions (e.g. time-dependent junction); record and send to 3-D model the pressure and temperature at this boundary.

To ensure the balance of pressure and velocity field, Picard iterations are applied to the coupling scheme. At each time step, the data exchange between 3-D model and 1-D model are iterated until the preset convergence criteria is reached.

Figure 2-2. Example of a non-overlapping 3D-1D flow coupling scheme in SAM. Data exchange happens in location 1 (core inlet) and location 2 (core outlet).

2.2 Conjugate Heat Transfer Modeling between Multi-Dimension Flow and Solid Structure

In pebble-bed nuclear reactor designs, either the traditionally gas-cooled or advanced molten salt-cooled, the side reflector is generally made of large graphite blocks in the shape of an annulus that surrounds the fuel pebble bed, as schematically shown in Figure 2-3 (a). Depending on the design, a central reflector is sometimes also used (not shown in Figure 2-3). Because of the generally very large volume, the graphite reflectors represent a large thermal inertia inside the reactor vessel of the reactor primary system. It is therefore critical for thermal-hydraulics analysis to capture the heat transfer between the fuel pebble bed and the reflectors. For normal operation conditions, this heat transfer is one of the main factors that determine the graphite reflector temperatures. For certain transients, such as the pressurized conduction cooldown (PCC) event of a typical pebble bed HTGR design, decay heat must be removed radially from the core to the side reflector, then to the outer surface of reactor vessel, and eventually to the reactor cavity cooling system (RCCS). The heat transfer coefficient between the pebble bed and the reflectors is an important parameter that affects the accurate prediction of core temperatures during such transients.

Figure 2-3. (a) A schematic drawing of pebble bed reactor core, including both the fuel pebble bed and the side reflectors; (b) A schematic drawing of heat transfer between the pebble bed and the side reflector.

The wall-to-pebble-bed heat transfer had been the subject of several past studies, from which empirical correlations were proposed, such as the Yagi and Wakao correlation [3] and the Achenbach correlation [4]. When deriving these correlations, for example, the Yagi and Wakao correlation [3], assumptions were made that the fluid and particle phase were at thermal equilibrium. The wall-to-pebble-bed heat transfer is due to the temperature difference between the bed and the wall on the wall-to-pebble-bed interface, and the heat transfer coefficient is lumped into a single parameter analogy to the classic convective heat transfer coefficient between a wall and a flow field. Yagi and Wakao [3] found that the wall-to-pebble-bed heat transfer coefficient was not sensitive to the thermal conductivity of the solid pebble, and it could

be correlated to fluid thermophysical properties, e.g., thermal conductivity and Prandtl number of the fluid, and fluid flow properties, e.g., Reynolds number. Because their data were obtained using air as the only working fluid, Prandtl number effect was not included for the correlation fitting, and its effect was later included using the so-called ‘*J* factor’ (refer to the Yagi and Wakao [3] for more detailed discussion). The Yagi and Wakao correlation for the wall-to-pebble-bed heat transfer coefficient, h_w , is given as:

$$\frac{h_w}{c_p \rho u} Pr^{2/3} = 0.2 Re_p^{-0.2},$$

where $Pr = c_p \mu / k$ is the Prandtl number of the fluid; and $Re_p = \rho u d_p / \mu$ is the modified Reynolds number based on the particle (pebble) diameter d_p ; and ρ , k , μ and c_p are the density, thermal conductivity, dynamic viscosity, and specific heat of the fluid, respectively. u is the superficial velocity of the fluid. Using the conventional definition for the Nusselt number, i.e.,

$$Nu_w = \frac{h_w d_p}{k},$$

Yagi and Wakao correlation could be rewritten in terms of wall Nusselt number as:

$$Nu_w = 0.2 Re_p^{0.8} Pr^{1/3}$$

Yagi and Wakao [3] suggested that the correlation is valid for $Re_p > 20$.

The Achenbach correlation [4] is quite similar to the Yagi and Wakao correlation, but it further considers the pebble-bed-diameter (d_{bed}) effect. The Achenbach correlation is given as:

$$Nu_w = \left(1 - \frac{d_p}{d_{bed}}\right) Re_p^{0.61} Pr^{1/3}$$

The recommended valid region of the Achenbach correlation is $50 < Re_p < 2 \times 10^4$ [4].

It is worth noting the inconsistent assumptions used in the derivation of these wall-to-pebble-bed heat transfer coefficients and those used in SAM’s porous-medium flow model. As discussed earlier in this section, it was assumed that the fluid and the pebbles were at thermal equilibrium when deriving the Yagi and Wakao correlation. This is however not the case for SAM’s porous-medium flow model, which assumes thermal non-equilibrium between the two components. Consequently, SAM’s porous-medium flow model includes an energy equation for the fluid phase and an additional energy equation for the solid pebble phase [2][5]. This is a necessary treatment for core thermal-hydraulics analysis for pebble bed reactor, where heat is generated in the fuel pebbles and fluid is the cooling medium. To address such an inconsistency, additional assumption must be made. Yagi and Wakao argued that there are two main heat transfer mechanisms near the wall, i.e., the wall-to-pebble heat transfer and the wall-to-fluid heat transfer, schematically shown in Figure 2-3 (b), and the former mechanism only made little contribution compared to the later one. The argument was made based on their experimental conditions, where the flow was in turbulent flow conditions. Following a similar reasoning, in SAM’s porous-medium flow model, we argue that the wall-to-pebble-bed heat transfer coefficient can be solely used to model the heat transfer between the wall and the fluid phase, i.e., $q''_{wall} = h_w (T_w - T_f)$. Regarding the solid pebble energy equation, two possible boundary conditions could be used at the wall-to-pebble-bed interface. The first option is the zero-heat flux boundary condition, which conserves the total wall-to-pebble-bed heat transfer, combined

with the assumption that all wall-to-pebble-bed heat flux goes to the fluid phase. However, this option results a discontinuous solid phase temperature across the wall-to-pebble-bed interface, which does not seem to be physical as the pebbles are in direct contact with the solid wall. The second option is to assume a continuous solid phase temperature across the same interface, which remove the non-physical temperature jump, and is used in the simulations discussed later in this report.

The implementation of the wall-to-pebble-bed heat flux relies on the so-called ‘InterfaceKernel’ of the MOOSE framework, which is able to set boundary conditions to internal boundaries (interfaces) of a simulation domain. A recent coordinated code development between SAM code development team and the MOOSE team created a dedicated ‘ConjugateHeatTransfer’ MOOSE object in the ‘Heat Conduction’ module for the general-purpose wall-to-fluid heat transfer. To illustrate the code implementation, considering the following fluid energy equation and pebble-bed solid phase energy equation [2][5]:

$$\begin{aligned} \varepsilon \rho c_p \frac{\partial T_f}{\partial t} + \rho c_p \vec{v} \cdot \nabla T_f - \nabla \cdot (\varepsilon k_f \nabla T_f) - q''' + a_w h (T_f - T_s) &= 0, \\ (1 - \varepsilon) \rho_s c_{p,s} \frac{\partial T_s}{\partial t} - \nabla \cdot (k_{eff} \nabla T_s) + a_w h (T_s - T_f) - q''' &= 0. \end{aligned}$$

as well as the solid phase energy equation for the reflector,

$$\rho_R c_{p,R} \frac{\partial T_R}{\partial t} - \nabla \cdot (k_R \nabla T_R) = 0.$$

Here, we use the subscripts f , s , and R for the fluid phase, the solid pebble phase, and the reflector solid phase, respectively. More details on the different terms of these equations can be found in references [2] and [5], and details on MOOSE implementation of the equation, including boundary conditions, are referred to reference [2]. As schematically shown in Figure 2-4, the simulation domain consists of the pebble bed domain (block 1) and the reflector domain (block 2), between which an interface exists. The fluid temperature and solid pebble temperature are only defined in block 1, and the reflector temperature is only defined in block 2. Correspondingly, MOOSE ‘kernels’ are added in block 1 for the fluid energy and pebble energy equations, and in block 2 for the reflector energy equation. On the interface, as discussed previously, we have the following conditions:

$$T_s = T_R \text{ and } q''_{wall} = h_w (T_R - T_f)$$

The first condition can be easily satisfied in the MOOSE framework using continuous finite element method, if a same variable is defined in both blocks 1 and 2 for the solid phase temperatures (both pebble and reflector). The second condition is implemented in the ‘ConjugateHeatTransfer’ InterfaceKernel, which assigns a boundary condition to the fluid phase energy equation, i.e., $q''_{wall} = h_w (T_R - T_f)$, and adds the same heat flux contribution to the boundary condition of the reflector energy equation. This results an additional condition on the interface:

$$-k_R \frac{\partial T_R}{\partial x} = -k_{eff} \frac{\partial T_s}{\partial x} + h_w (T_f - T_R)$$

which is exactly the require energy balance across the interface.

Figure 2-4. Variables arrangements and the pebble-bed and reflector blocks.

3 Reference FHR Model Development

In order to demonstrate and evaluate the ability of SAM to model a pebble-bed fluoride-salt-cooled, high temperature reactor (PB-FHR), a generic primary loop was developed. The PB-FHR primary loop consists of a core model, salt pump, expansion tank, helical heat exchanger, and the supporting piping. The generic model is based on the University of California, Berkeley (UCB) Mk1 design [7], but removes some of the novel characteristics that are unlikely to be present in early commercial designs. These characteristics include the central reflector region, and the graphite reflector pebbles at the periphery of the core. A graphical representation of a PB-FHR core, after accounting for these changes, is shown in Figure 3-1. Note, this representation is not to scale.

Figure 3-1. Graphical representation of a generic PB-FHR, including the downcomer, pebble bed core, salt collection ring, defueling chute and salt extraction pipe.

As shown in Figure 3-1, cold salt is assumed to flow downward between the graphite reflector (core barrel not included in the simulation) and the reactor vessel wall. After being collected in the inlet plenum at the bottom of the reactor core, the cold salt is forced upwards through a packed pebble bed reactor core. At the top of the core, hot salt is forced radially outward into a salt collection ring, while the fuel pebbles slowly travel upwards through the defueling chute. The movement of the fuel pebbles is however not considered in the simulations discussed in this report. After being collected in the outer ring, the salt is extracted through a pipe. Due to a lack of information, bypass flow, which is expected within the graphite reflector, is currently neglected.

The dimensions of the reactor core are based on the thermal hydraulic studies presented in reference [7]. The pebble bed core can be decomposed into four regions, a fueling chute, a cylindrical region, a contraction region and a defueling region. In order to simplify the geometry, it has been assumed that the active core does not extend past the cylindrical region, hereafter referred to as the active core. The defueling chutes are also lumped into the top graphite reflector, since they only occupy relatively small volumes and the flow inside is close to be stagnant. The axial and radial boundary of each region are shown in Figure 3-2. The total volume of each segment is summarized in Table 3-1.

Figure 3-2. Dimensions of a generic PB-FHR reactor core.

Table 3-1 Total volume within each section of a PB-FHR core.

Core Region	Total Volume [m ³]
Fueling Chute	3.0478
Active Core	8.6590
Contraction Section	1.4082
Defueling Chute	0.7238*

* The total volume of the defueling chute only accounts for the section of the defueling chute contained within the graphite reflector.

The volume of the fuel present within the reactor core is based on an average porosity of 0.4. The fuel pebbles are composed of a graphite center, a fuel matrix, and an outer graphite shell. The thickness of the graphite center, fuel matrix and outer shell are 1.25 cm, 0.15 cm and 0.1 cm, respectively. The resulting fuel pebble outer diameter is 0.03m. The average power density of the core is assumed to be 24.4 MW/m³, resulting in a total thermal power of 320 MW. The inlet temperature is assumed to be 550 °C with an outlet temperature of 650 °C. The corresponding flow rate is 1324.6 kg/s.

The primary loop, shown in Figure 3-3, is based on the Mk1 SAM model presented in reference [8]. 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. In order to prevent the primary salt velocity from exceeding 2 m/s, an identical second primary loop is introduced.

Figure 3-3. Graphical representation of the PB-FHR primary system.

3.1 Core Modeling Demonstration

3.1.1 2D Core Model Development

Using the core geometry shown in Figure 3-2, a 2-D mesh was created using CUBIT [9]. The mesh, shown in Figure 3-4, 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 the mixture of a coolant and a solid. This 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, block 4 and upper reflector, block 2 and 3, are modeled as a solid zone due to limited information on the flow paths within each zone.

Figure 3-4. 2-D PB-FHR mesh with block (left) and boundaries (right) labeled.

The fluid within blocks 11, 12, 13, and 15 are subject to the porous-medium flow equations [2][5]. The friction factor is determined using the KTA correlations, a well-validated correlation commonly used in HTGR thermal-hydraulics analysis, which also demonstrated very good accuracies against several sets of selected experimental data in our previous validation study [10]. Heat transfer between the fluid and solids within the porous blocks follows Newton's law of cooling, with the heat transfer coefficient determined using the KTA correlation (see discussions and references provided in [5]). The volumetric heat generation rate is defined within the solids in block 12, the active core. At the interface of the porous zones and the solid zones, boundaries 3, 4, and 11, the heat transfer coefficient is determined using the Achenbach correlation (see section 2.2). The core inlet conditions, temperature and velocity, are defined at boundary 1. The core outlet condition, pressure, is defined at boundary 14. All remaining boundaries are assumed to have a no heat flux boundary condition, including boundaries 6 and 7. This assumes that the heat transfer from the graphite to the supporting materials and inlet plenum is negligible. Further studies are needed to justify this assumption.

3.1.2 2D Core Model Steady State Results

Using a core inlet temperature of 823.15 K (550 °C), an inlet superficial velocity of 0.4032 m/s, and an outlet pressure of 0.12 MPa, a null transient is run until the 2-D core reaches a steady state. During the null transient all boundary conditions are held constant and the volumetric heat rate within the active core region is held at 37 MW/m³.

The coolant and solid temperature profiles of the generic PB-FHR are shown in Figure 3-5. The velocity magnitude and pressure profile are shown in Figure 3-6. The coolant temperature contains a gradual increase from the inlet temperature to the outlet temperature beginning at the lower boundary of the active core. The solid temperature, which includes the fuel pebbles and graphite reflector, follows a similar trend as the coolant temperature but the maximum temperature is slightly higher, 950 K compared to the 923 K coolant temperature. Due to the adiabatic boundary conditions on the exterior graphite surfaces, the steady state reflector temperature closely follows the bulk coolant temperature. In order to better capture the temperature gradient that will develop within the graphite reflector, the bypass flow within the reflector should be considered. Heat transfer to the core barrel, downcomer and inlet plenum will also affect the temperature gradient within the reflector. This effect can be captured by incorporating the core barrel, downcomer and inlet plenum using SAM *PBOneDFluidComponent*, and *PBVolumeBranch* components.

Figure 3-5. Steady state coolant (left) and solid (right) temperatures.

Figure 3-6. Steady state velocity magnitude (left) and pressure (right).

3.2 1-D Primary System Modeling Demonstration

Using the primary system geometry shown in Figure 3-3, a 1-D SAM model was developed. The reactor core was modeled using a single channel approach. The single channel contains 367,500 fuel rods representing the fuel pebbles stacked one on top of the other. The thickness of each region within the fuel rod is set such that it conserved the mass of each pebble region. The total surface area for a stack of pebbles was conserved by scaling the heat transfer coefficient by the ratio of the stacked pebble surface area to the cylindrical rod surface area.

The orifice coefficient of the collection ring inlet was tuned such that the 1-D pressure drop across the core matched the 2-D pressure drop across the core. The remainder of the primary loop was model using a series of *PBPipe*, *PBBranch* and *PBVolumeBranch* components. A single loop with a flow area multiplicity of two was used to represent the two-loop system in order to reduce the complexity of the model. The pump head was calibrated such that the flow rate within the primary system reached the steady state value of 1324.6 kg/s. A pump head of 0.44 MPa achieved this value.

The steady state coolant temperature within the primary loop is shown in Figure 3-7. Heat loss to the environment is not considered. The heat exchanger was designed such that the correct inlet and outlet temperatures were achieved at steady state. The properties for the secondary salt, “solar” salt, were obtained from [11]. The primary salt is assumed to be on the tube side of the heat exchanger. There are 1208 primary tubes with an inner diameter of 1.96 cm and a total flow length of 18.47 m. The shell side of the heat exchanger has a length of 3.418 m and a flow area of 0.2 m². The “solar” salt enters the heat exchanger at 700.15 K with a mass flow rate of 5,060 kg/s. At this time, SAM is not able to graphically represent a helical tube (while

conserving the length and height of the helical tube), as a result the temperature profile shows a discontinuity at the end of the heat exchanger. This discontinuity is not present within the 1-D model and is simply an artifact of the visualization software.

Following the steady state calculation, a protected loss of forced convection (PLOFC) accident was simulated. Beginning at 250 seconds, the power to the primary coolant pump is lost, and the reactor core is scrammed. The reactor core is assumed to follow a standard decay heat curve, while the primary coolant pump is assumed to have a pump coast down time of 4.5 seconds. The flow rate on the secondary side of the primary heat exchanger is assumed to follow a coast down curve similar to the primary pump, however, unlike the pump head, the secondary coolant flow decays to a mass flow rate of 632.6 kg/s, not zero. The time history of the reactor power and primary coolant pump is shown in Figure 3-8. The transient was run for 2500 seconds.

The core inlet and outlet temperature, flow rate and maximum fuel surface temperature following the transient are shown in Figure 3-9, Figure 3-10 and Figure 3-11, respectively. The core flow rate decreases quickly, until a natural circulation flow rate of 21 kg/s is established. As the flow rate decrease, the coolant residence time outside the reactor core increase. As a result, the core inlet temperature remains relatively constant until approximately 1000 seconds. At this time, the core inlet temperature quickly drops due to overcooling in the heat exchanger. At the beginning of the transient, the core outlet temperature rises gradually due to the decreased flow rate. As the transient progresses, the core outlet temperature follows the decreasing trend of the core inlet temperature. As the core outlet temperature decreases, the exit temperature of the heat exchanger will also decrease, eventually leading to freezing in the primary loop. Based on the core inlet temperature, freezing is assumed to occur around 2,250 seconds.

Figure 3-7. Primary loop coolant temperatures at steady state.

Figure 3-8. Evolution of the reactor power (top) and primary pump head (bottom).

Figure 3-9. 1-D core inlet and outlet temperature following a postulated PLOFC.

Figure 3-10. 1-D core flow rate following a postulated PLOFC.

Figure 3-11. 1-D maximum fuel surface temperature following a postulated PLOFC.

3.3 Coupled 2-D/1-D Primary System Modeling Demonstration

Using the 2-D core model presented in Section 3.1 and the 1-D primary system model presented in Section 3.2, a 2-D/1-D coupled PB-FHR model was created. The 2-D/1-D model utilizes the Moose MultiApp structure outlined in Section 2.1, Figure 2-2. The 1-D primary

model replaces the core channels, outlet plenum, and part of the extraction pipe with two boundary conditions, one at the core inlet and one at the core outlet. The 2-D core model remains largely unchanged, but includes additional MultiApp and Transfer blocks that drive the coupled simulation and allow the 2-D and the 1-D models to exchange data at each interface. At the core outlet, the 2-D model sends the average velocity magnitude and average temperature and receives the pressure. At the core inlet, the 1-D model sends the velocity and temperature and receives the pressure.

In order to promote solution stability at both interfaces, Picard iterations are enabled during the transient solve. The relative convergence and absolute convergence criteria for the Picard iterations is set to $1\text{E-}4$, and $1\text{E-}3$, respectively. A Picard relaxation factor of 0.2 is applied to all of the 2-D system variables and the maximum number of Picard iterations is set to 10. In the case that the Picard iterations do not converge, the solution is allowed to advance.

A three-step process is suggested to ensure the 2-D/1-D model achieves a steady state solution before running transient simulations. In the first step, the 2-D and 1-D models perform a zero-transient using the MultiApp framework, but no data is transferred at the interfaces. In this step, the 2-D/1-D model is effectively uncoupled, and each model is allowed to reach a steady state independently. This step can be accelerated by loading the steady state solution from the standalone models. In the second step, the 2-D/1-D model is restarted, and the zero-transient is continued, however, data is now transferred at the interfaces. The 2-D/1-D model can now be considered fully coupled. At the end of step 2, the 2-D/1-D model has reached a steady state, shown in Figure 3-12, and the solution can be used in the third step as the initial condition for a transient simulation.

The steady state surface temperature of the fuel pebbles in the 1-D and 2-D models show a small discrepancy of $6\text{ }^{\circ}\text{C}$. While the surface temperatures are in good agreement, the energy stored within the fuel is quite different due to the assumption used in the current porous medium formulation for the 2-D fuel pebble. It cannot correctly capture the peak and average solid temperatures, but only represents the solid surface temperature. As a result, the transient predictions of the 2-D model will show significant deviation from the 1-D model. Further work is required to better capture the stored energy within a fuel pebble when using the 2-D porous medium model.

Figure 3-12. Coupled 2-D/1-D temperature profile at steady state.

4 Water-based NSTF Cavity Modeling with SAM

The Natural convection Shutdown heat removal Test Facility (NSTF) is a large-scale thermal-hydraulics test facility built at Argonne National Laboratory to study the performance of passive safety systems for advanced nuclear reactors [12]. It was designed to provide high-quality experiment data for validating the performance of Reactor Cavity Cooling System (RCCS) concepts for decay heat removal in advanced nuclear reactors. The heat removal in NSTF relies on natural convection cooling with either air- or water-based systems. The air-based NSTF testing program was successfully concluded in FY16. The current effort in NSTF testing program focus on water-based RCCS concept [13]. This section documents the modeling and computational analysis of RCCS in water-based NSTF with SAM's multi-dimensional flow module [2]. This effort also assists in evaluating SAM capabilities for safety analysis of FHRs, which may rely on RCCS for emergency decay heat removal.

4.1 SAM Model Description

The water-based NSTF cavity is modeled with SAM with a focus on the hot side of the cavity. Figure 4-1 shows the schematic of the cavity design. The hot side consists of the heated wall, adiabatic wall, water tube, water tube wall, cooling fin wall, and the cavity.

Figure 4-1. Schematic of water-based NSTF cavity: top-left (top view), top-right (exploded view of different blocks), bottom-left (vertical cut view through water tube), bottom-right (vertical cut view through fin)

At this stage, only the hot side cavity is modeled in 2-D to reduce computational cost. The schematic of the 2-D model is shown in Figure 4-2. The current model consists of 3 separate domains: heated wall, cavity, and the water tube wall. Different with the common CFD practice where the solid domains and the fluid domains are combined, the current model contains separate domains (and thus separate boundary surfaces) due to the necessity to consider the radiation heat transfer between the heat wall surface and the water tube wall surface.

Figure 4-2. Sketch of 2D hot side cavity model in SAM

The current model is featured with the following heat transfer modes:

- Q_{in} : Q_{in} specifies the external heating power supplied to the system. It is applied to the heated wall as the heat flux boundary condition. A uniform value of $Q_{in} = 3839 \text{ W/m}^2$ is used in the current simulation.
- Q_1 : Q_1 models the heat flux from the heated wall left surface to the cavity right surface. In the current model, a gap conductance model with a very high gap conductance ($h_1 = 10^6 \text{ W/(m}^2\text{K)}$) is used between these two surfaces. This setup models a negligible temperature drop between the two surfaces.
- Q_2 : Q_2 models the heat flux from the cavity left surface to the water tube wall. In the current model, a gap conductance model with a very high gap conductance ($h_2 = 10^6 \text{ W/(m}^2\text{K)}$) is used between these two surfaces. This setup models a negligible temperature drop between the two surfaces.
- Q_3 : Q_3 models the radiation heat transfer between the heated wall left surface and the water tube wall right surface. The emissivity of these two surfaces are listed in Table 4-2 and Table 4-3.

- Q_{out} : Q_{out} models the convective heat transfer between the water tube wall and the cooling water. In the current model, the water temperature is provided as an input function. The inlet temperature is fixed at 303.15 K and the water temperature is increased linearly along the axial direction with a total of 15 K temperature increase. A constant heat transfer coefficient of $h_c = 357.25 \text{ W/(m}^2\text{K)}$ is used. Note that this is a rather simple modeling of the heat transfer between the water tube wall and water. However, it provides the interface for the following coupled simulations where the 2-D cavity model will be coupled with the water loop and SAM's built-in heat transfer correlations will be used to calculate the heat transfer coefficients.

The geometry and material properties of hot side cavity, heated wall, the water tube wall, and the cooling fin are listed in Table 4-1, Table 4-2, Table 4-3, and Table 4-4, respectively [12][13].

Table 4-1 Geometry and material property of hot side cavity

Parameters	Values	Comments
Height	6.736 m	In z-direction
Width	1.32 m	In y-direction, not modeled in 2-D model
Depth	0.889 m	In x-direction
Material	Air	AirEquationOfState (incompressible)

Table 4-2 Geometry and material property of heated wall

Parameters	Values	Comments
Emissivity	0.78 - 0.79	0.78 is used
Thickness	0.0254 m	1 in
Material	SAE 1020 low carbon steel	
Density	7870.0 kg/m ³	1.0 for steady-state
Specific heat capacity	486.0 J/kg/K	
Thermal conductivity	51.9 W/m/K	

Table 4-3 Geometry and material property of water tube

Parameters	Values	Comments
Outer diameter	4.826E-02 m	1.90 in
Inner diameter	3.396E-02 m	1.337 in
Thickness	7.137E-03 m	0.281 in
Material	316L SS	
Emissivity	0.43	with processing
Density	8000.0 kg/m ³	1.0 for steady-state
Specific heat capacity	502 J/kg/K	
Thermal conductivity	16.00 W/m/K	

Table 4-4 Geometry and material property of cooling fin

Parameters	Values	Comments
Thickness	7.950E-03 m	0.313 in
Half thickness	3.975E-03 m	
Material	1018 Carbon steel	
Emissivity	0.43	with processing
Density	7832 kg/m ³	
Specific heat capacity	434 J/kg/K	
Thermal conductivity	51.9 W/m/K	

4.2 Turbulent Viscosity from STAR-CCM+ Simulation

Turbulent model is needed for a reasonable prediction of the flow field in the cavity, which is however limited in the current SAM multi-dimensional flow model. In this test, the turbulent viscosity from STAR-CCM+ 3-D simulation [14] is extracted and applied to SAM 2-D model. Figure 4-3 shows the profile of turbulent viscosity obtained from STAR-CCM+ simulation. The results from STAR-CCM+ 3-D simulation will be denoted as CFD results in the following discussion.

Figure 4-3. Turbulent viscosity from CFD simulation.

4.3 Base Simulation Results

Three levels of meshes are currently explored in SAM 2-D model, denoted as coarse, medium, and fine in the following discussions. The coarse, medium, and fine meshes have 3840, 14080, and 20480 elements, respectively. Figure 4-4 and Figure 4-5 show the fluid velocity magnitude and vertical fluid velocity in the hot side cavity. The comparison with same results from STAR-CCM+ is also included in these figures. It is seen that the velocity field from SAM 2-D model prediction is in good agreement with STAR-CCM+ result, except near the bottom and top boundaries. It is seen that the coarse mesh is generating chaotic feature near the top boundaries. The results with medium and fine mesh are much smoother and agree better with the results from STAR-CCM+ simulation.

Figure 4-4. Cavity fluid velocity (magnitude) at quasi steady-state. From left to right: SAM Coarse, SAM Medium, SAM Fine, and CFD

Figure 4-5. Cavity fluid velocity (z-direction) at quasi steady-state. From left to right: SAM Coarse, SAM Medium, SAM Fine, and CFD

Figure 4-6. Cavity fluid temperature at quasi steady-state. From left to right: SAM Coarse, SAM Medium, SAM Fine, and CFD

Figure 4-7 shows the fluid velocity along the axial mid-plane and comparison with STAR-CCM+ result. It is seen that the velocity from SAM prediction is close to STAR-CCM+ prediction, which is directly related to the turbulent viscosity profile. Figure 4-6 and Figure 4-8 shows the fluid temperature in the cavity from SAM prediction and STAR-CCM+ prediction. The profile of fluid temperature is seen to be similar, however, the SAM 2-D model underpredicts the bulk fluid temperature and the heated wall temperature, see Figure 4-9. This is caused by the incorrect prediction of convective heat transfer and radiation heat transfer flux, which will be analyzed in a calibration study in the following section.

Figure 4-7. Cavity velocity magnitude (left) and vertical velocity (right) at the axial mid-plane

Figure 4-8. Cavity temperature at the axial mid-plane.

Figure 4-9. Solid temperature at the cavity left and right wall

Table 4-5 NSTF Cavity heat balance results

Quantity	Mode	Coarse: W/m (%)	Medium: W/m (%)	Fine: W/m (%)
Q_{in}	External heat input	25859.1 (100.0)	25859.1 (100.0)	25859.1 (100.0)
Q_1	Convective heat to cavity	8000.8 (30.9)	5208.3 (20.1)	4968.8 (19.2)
Q_2	Convective heat to tube wall	9029.0 (35.0)	5840.2 (22.5)	5176.0 (20.0)
Q_3	Radiation heat to tube wall	17872.7 (69.1)	20736.8 (80.1)	20956.8 (81.0)
$Q_1 + Q_3$	Total heat to tube wall	25873.6 (100.0)	25945.1 (100.2)	25925.6 (100.2)
Q_{out}	Heat out to water	26886.4 (104.4)	26341.1 (101.8)	26138.3 (101.1)

Table 4-5 lists the heat balance analysis for results from 3 levels of meshes. As a reference, the percentage of convective heat flux from STAR-CCM+ simulation is about 20.4% (it varies with locations). The heat balance results show that the convective heat flux with the coarse mesh is over predicted (30.9% vs 20.4%), while the convective heat flux with the medium and fine mesh are much closer (20.1% vs 20.4%). It is also seen that the heat balance (Q_{out} vs Q_{in}) in the coarse mesh is worse. This indicates that the coarse mesh is not fine enough to capture the correct flow behavior.

From the mesh sensitivity analysis results reported in this section, it is seen that the medium mesh is fine enough to capture the major flow profile. In the following study, the medium mesh will be used.

4.4 Calibration Study Results

It is seen that SAM 2-D model under-predicts the bulk fluid temperature and heated wall temperature, which is likely caused by the simplification to the radiation heat transfer. In SAM 2-D model, radiation heat transfer is modeled between the heated wall and the tube wall, which is essentially the radiation transfer between two parallel plates. However, in STAR-CCM+ 3-D model, the adiabatic walls are also modeled with radiation heat transfer and have smaller emissivity, i.e. 0.2 for the side walls and 0.005 for top/bottom walls. This simplification makes SAM 2-D model more effective in radiation heat transfer, i.e. the heated wall temperature is much lower to transfer the total heat. In order to estimate and compensate for this simplification effect, a calibration study is performed with respect to the radiation heat transfer and convective heat transfer models.

The radiation heat transfer between heat structures walls are simulated in SAM by:

$$Q_{rad} = \frac{\sigma}{\left(\frac{1}{\epsilon_1} - 1\right) + \frac{1}{f_{view}} + A_r\left(\frac{1}{\epsilon_2} - 1\right)} (T_1^4 - T_2^4) = h_{rad}(T_1^4 - T_2^4)$$

with

$$h_{rad} \equiv \frac{\sigma}{\left(\frac{1}{\epsilon_1} - 1\right) + \frac{1}{f_{view}} + A_r \left(\frac{1}{\epsilon_2} - 1\right)}$$

where σ , ϵ_1 , ϵ_2 , f_{view} , and A_r are the Boltzmann constant, emissivity of first wall, emissivity of second wall, view factor, and area ratio, respectively. h_{rad} is introduced as an effective radiation heat transfer coefficient, which is completely determined by ϵ_1 , ϵ_2 , f_{view} , and A_r . For SAM's numerical simulations, modification to any of ϵ_1 , ϵ_2 , f_{view} , and A_r is equivalent to modification to h_{rad} .

In the first step of the calibration study, a multiplier (ϕ_{rad}) will be applied to h_{rad} to study the effect of radiation heat transfer to the simulation results, mainly the bulk fluid temperature and heated wall temperature. In this calibration test, $\phi_{rad} = 0.55$ is used. The result is shown in in Figure 4-10 and Figure 4-11.

With $\phi_{rad} = 0.55$, it was observed that through heated wall temperature from SAM prediction is closer to the STAR-CCM+ prediction, but the bulk fluid temperature is still underestimated. Besides, because the radiation heat transfer is reduced, the radiation heat flux is also reduced, which is not desired. A second calibration study is performed to the gap conductance between the solid wall and cavity (i.e. h_1 and h_2), to increase effectively the heat resistance of convective heat transfer. In this calibration step, the gap conductance of $h_1 = 100.0 \text{ W}/(\text{m}^2\text{K})$ and $h_2 = 10.0 \text{ W}/(\text{m}^2\text{K})$ are used. This will introduce non-negligible temperature drops between the fluid temperature and solid temperature at the right and left surface, respectively. h_1 and h_2 are not equal considering that the effective convective heat transfer in heating and cooling surface are physically different. The results are shown in Figure 4-10 and Figure 4-11. The additional temperature drops between fluid and solid in the cavity left (cooling surface) and right surface (heating surface) are 87.9 K (due to h_2) and 7.96 K (due to h_1), respectively.

Figure 4-10. Cavity temperature at the axial mid-plane with/without calibration. Only calibration II will introduce a non-negligible temperature drop between the fluid temperature and wall temperature near the boundary.

Figure 4-11. Fluid temperature along lateral midplane with/without calibration (left); cavity right wall temperature with/without calibration (right)

4.5 Coupled Simulation Results

In the previous study, the cooling water was not directly simulated and a constant tube wall to cooling water heat transfer coefficient was used. In this section, the cooling water is simulated by SAM's 1-D component and then coupled with SAM 2-D cavity model. The SAM 1D-2D coupled simulation is performed in preparation for the planned TRACE-SAM coupling case when it is ready. It is planned to use TRACE to model the NSTF water loop, and to run coupled SAM-TRACE simulation of the NSTF test.

The coupling scheme is based on the convective heat transfer between the cooling tube wall and the cooling water. The MOOSE's MultiApp system is used and Picard iteration is applied between the main model (SAM 2-D cavity model) and the sub model (SAM 1-D cooling water model). The physical and boundary conditions of the SAM 1D cooling water model are listed in Table 4-6. The heated perimeter is calculated based on the heat balance, i.e. the total heat input is carried out by the 8 cooling water channels, more specifically it is the ratio of width of cavity (i.e. 1.32 m) and number of cooling water channels (i.e. 8).

Table 4-6 Physical and boundary conditions for SAM 1-D cooling water model

Parameters	Value	Parameter	Value
Height	6.736 m	Mass flow rate	0.0675 kg/s
Area	9.057e-4 m ²	Inlet temperature	303.15 K
Hydraulic diameter	3.396e-2 m	Inlet velocity	0.075 m/s
Heated perimeter	0.165 m	Outlet pressure	10 ⁵ Pa

The coupled simulation starts from the calibration result obtained previously. The SAM 2-D cavity model and SAM 1-D cooling water model are coupled to perform a null-transient simulation until the steady-state is reached, i.e. the heat is balanced. The results are shown below. Figure 4-12 shows the transient outlet cooling water temperature and the heat flux output to cooling water in the null-transient simulation. Figure 4-13 shows the steady-state water temperature and the tube wall inner surface temperature. Because the physical conditions are

setup the same as in the base case simulation, the water temperature increase roughly linearly from the inlet to outlet with a total temperature increase about 15 K, which is similar to the preset temperature increase in previous simulation studies. The result in the cavity is very close what was shown in previous Sections, and is thus ignored here.

Figure 4-12. Outlet water temperature (top) and heat balance (bottom) during the coupled null-transient simulation

Figure 4-13. Cooling water and tube wall inner surface temperature

5 Summary

The molten-salt-cooled pebble-bed reactor, or pebble-bed FHR (PB-FHR) is a promising candidate among advanced nuclear reactor concepts with its improved passive safety characteristics and high thermal efficiency. To support the development and utilization of the SAM code for molten-salt-cooled pebble-bed reactor safety analysis and licensing, a reference primary loop model of PB-FHR is developed, based on the UC Berkeley Mk1 FHR design and incorporated some design features in Kairos Power's KP-FHR core.

At first, a standalone reference primary loop model was developed using SAM's one-dimensional flow module, with the reactor core modeled by a single channel approach. Steady-state and transient simulations were demonstrated with this standalone reference model. Then, a coupled 1D-2D reference model was developed, which leverages the latest improvements on multi-dimensional flow modeling and 1D-3D coupling techniques in SAM. The PB-FHR core is modeled by a two-dimensional porous medium while the external circuits are represented by a one-dimensional SAM model for efficient calculation. A reference standard problem of the reactor primary loop model is foundational to the methodologies employed by NRC to verify the adequacy of computer codes and evaluation models. It has been successfully demonstrated that SAM can be used in modeling the complete PB-FHR primary loop with the multi-D/1-D coupling techniques and the conjugate heat transfer between porous medium core and the solid reflector.

A separate study was also performed on SAM simulation of the water-based NSTF cavity, which assists in evaluating SAM capabilities for modeling the emergency heat removal systems relying on RCCS concepts. The water-based NSTF cavity is modeled using SAM multi-dimensional flow module. SAM simulation results were benchmarked with results from STAR-CCM+ 3-D simulations. It is found that the velocity field from SAM 2-D model prediction is in very good agreement with the STAR-CCM+ simulation result. The profiles of fluid temperatures are similar; however, the SAM 2-D model under-predicts the bulk fluid temperature and the heated wall temperature. Through calibrations of radiative heat transfer and solid-liquid interface heat transfer parameters, very good agreements between SAM and STAR-CCM+ simulation results can be achieved.

Meanwhile, several technical challenges are identified in this work:

1. The current 1D/multi-D coupling strategy still requires further improvements. While the coupling scheme is working well, the performance needs improvements. It currently requires a large number of Picard iterations to ensure the consistency at the coupling interfaces, and the use of small under-relaxation factors in Picard iteration to avoid numerical stability or convergence issues during transient simulations.
2. An efficient yet adequately accurate turbulence modeling capability is desired in SAM. The turbulent viscosity data from high-resolution STAR-CCM+ simulations was used in SAM simulations of NSTF cavity to improve the accuracy of the results. To preserve SAM's excellent efficiency while improving the fluid solution accuracy, novel reduced-order models will be pursued (instead of the implementation of traditional turbulence models).
3. The current porous medium model cannot correctly capture the peak and average solid temperatures. As a result, the stored energy in the solid would be incorrect; thus, the transient responses of the porous medium model could show significant deviations.

Note the solid temperature calculated in the current porous medium formulation only represents the solid surface temperature.

In light of the challenges listed above, continuous study will focus on addressing these limitations and further expanding SAM's modeling capabilities for PB-FHR design needs. In addition, the primary loop model will be integrated with a RCCS decay heat removal system; and the whole system transient simulations are to be performed to study the PB-FHR system responses under postulated operational or accident scenarios. Lastly, coupled TRACE-SAM simulation will be performed for water-based NSTF tests in which the two-phase natural circulation flow in NSTF will be modeled by TRACE.

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