THERMAL ANALYSIS OF PEBBLE-BED REACTORS BASED ON A TIGHTLY COUPLED MECHANICAL-THERMAL MODEL

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ABSTRACT

In pebble-bed reactor designs, pebble flow and coolant flow interplay with each other by the interaction forces, normally the drag force or buoyancy force. This requires a tightly coupled simulation between pebble flow and coolant flow in order to provide accurate predictions of core dynamics. In realistic operations of pebble-bed reactors, the above interplay is further complicated by the heat transfer and resultant temperature distribution in the core. Temperature changes the pebble friction coefficient, pebble-coolant drag coefficient as well as the coolant viscosity, which all in turn affect the pebble flow and coolant flow thermal and dynamic behaviors. In this paper, we present a thermal analysis of a Fluoride-salt-cooled High-temperature Reactor (FHR) based on a tightly coupled mechanical-thermal model. Pebble flow is simulated using the discrete element method (DEM). The fission heating source, heat conduction, and temperature in each pebble are explicitly modeled. Coolant flow is simulated based on the computational fluid dynamics (CFD) method by solving time- and volume-averaged Navier-Stokes equations in a porous medium. Thermal heat transfer, pressure gradient, and temperature distribution in each control volume are calculated. Pebble-coolant interactions are modeled based on the experimentally fitted correlations, accounting for the temperature effect. The coupled model formulates a coupled DEM-CFD computational scheme that requires the information exchange at a certain frequency between two flow simulations. Based on an assumed power density distribution, we analyze a small scale FHR design and report the dynamic and thermal results. These results include volume-averaged pebble surface temperature distribution, the pebble packing density distribution over the whole core. Also, coolant temperature, pressure and velocity distribution over the whole core are reported.

KEYWORDS
pebble-bed reactor, mechanical-thermal coupling, granular flow, DEM-CFD, thermal heat transfer

1. INTRODUCTION

Pebble-Bed Reactor (PBR) designs present special interests to the nuclear energy community since their first deployment as a research reactor [1]. PBR design was proved experimentally to be fundamentally safe [1] although controversial arguments still exist. In past two decades, new reactor concepts based on pebble-bed design were continuously proposed, such as Pebble-bed Very High Temperature Reactor (PB-VHTR) [2], and some are actually built, e.g. HTR-10 design [3], or being constructed, e.g. HTR-PM [4]. These designs (PB-VHTR, HTR-10 and HTR-PM) use helium gas as coolant in the primary loop. As an alternative, the very recently proposed Pebble-Bed Fluoride-salt-cooled High Temperature Reactor (PB-

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FHR), which was called Advanced High Temperature Reactor (AHTR) earlier [5, 6], uses liquid salt as the coolant. FHR has many advantages compared with gas-cooled PBR, such as the ability to operate at high temperatures and low pressure, with higher power density than its helium-cooled counter-part. Current PB-FHR is still in concept evaluation stage [6, 7].

In PBRs, the solid phase (pebble flow) and the fluid phase exchange momentum and energy by fluid-pebble interaction force and fluid-pebble heat transfer, forming a coupled multi-physics system. For PB-FHR, the fluid-pebble interaction is the primary force (the density of the salt is higher than the graphite pebbles so the pebbles are floated around the coolant) that drives the pebble flow in the core and need to be considered in the core modeling and safety analysis in order to accurately understand the core dynamics. Previous effort by other researchers has been made to study the thermal-hydraulics of gas-cooled PBRs[2, 7-13], in which decoupled approaches are adopted where the pebble flow dynamics is separated from the coolant fluid dynamics. Pebble spatial distribution (packing fraction profile) is obtained by either a static porosity correlation [11-12] which neglect the slow pebble motion, or a single pebble phase modeling via Discrete Element Methods (DEM which tracks each pebble's motion for the thermal-fluids calculation [2, 7, 13]. The major assumption underlying the decoupled approach is that the pebble distribution is not affected by the fluid motion and its thermal dynamics, neglecting the fluid-pebble interaction effect on the pebble motion. For the PB-FHR case or the large scale gas-cooled PBR (such as PBMR400) case, the pebble-fluid interaction is strong enough such that the fluid force on a pebble is higher than pebble gravity, which calls for a multi-physics model that combines the pebble dynamics and fluid dynamics together [14, 15] . In our previous efforts, a multi-physics model has been developed to simulate the 3-D pebble flow in PBR designs accounting for the gas-pebble (HTR-10) or liquid-pebble (FHR) interactions [15]. Coupled pebble and coolant flow were simulated using a coupled Discrete Element Method and Computational Fluid Dynamics (CFD-DEM) model with high fidelity. The assumption of a constant temperature is adopted in previous work and heat transfer is not considered. This assumption is not accurate for a gas-cooled PBR, e.g. typical PB-VHTR designs, in which the density variation of the gas coolant is prominent with temperature. For FHR, although the molten salt is nearly incompressible and the temperature variation is much smaller than that of gas-cooled PBR, a realistic heat transfer model with temperature distribution is still necessary in order to accurately capture the mechanical behavior (such as friction) of the pebbles, which is temperature dependent.

The research efforts toward a fluid-particle flow system with temperature variations have been made in various applications [16-18], mostly for fluidized-bed applications and other chemical reactors. In this work, the multi-physics approach is applied in PB-FHR with heat transfer between the fluid and solid phases, allowing the temperature difference between coolant and pebbles. The DEM approach is still employed to solve the pebble motion in the new multi-physics model, owing to its capability to capture the pebble-fluid interaction effect with high fidelity. A small scale PB-FHR design with a similar geometric configuration of HTR-10 [9] is studied by analyzing the thermal-fluids and mechanical behavior of the system.

2. METHODOLOGY DESCRIPTION

The pebble-coolant force interaction (fluid momentum source term) mainly comes from the interphase drag, which is significant enough to alter the spatial distribution of packed bed and necessitates a coupled multi-physics modeling. The coupled model in the DEM-CFD approach is realized by adding a fluid-pebble interaction term in each flow's dynamic equations and introducing a fluid-solid heat transfer term in each flow's thermal equations. The equations of motion for the pebble flow are based on the Newton's law of motion. The contact forces between pebbles are determined by the Hertzian contact mechanics theory [19]. The ensemble-averaged coolant flow equations are based on fluid mass continuity, momentum and energy conservation. The inter-phase drag force and heat transfer models are based on experimentally established correlations.

For the proposed multi-physics model, since the dynamics of fluid and discrete solid phase evolve at different length and time scales [20], it is inefficient and unnecessary to solve the combined pebble-coolant equations at each time step. Instead, it is practical to adopt a tightly coupled solver which exchanges the fluid and particle information at a reasonable interval, and consequently greatly save computation time without loss of fidelity. In this section, the governing equations and models used in this work are introduced.

2.1. Coolant Flow Simulation Model with Thermal Heat Transfer

The fluoride salt is treated as incompressible liquid in this work. As in previous CFD-DEM approach, the ensemble-averaged mass and momentum balance equations of molten salt fluid can be written as

$$\frac{\partial \varepsilon}{\partial t} + \nabla \bullet (\varepsilon \bar{\boldsymbol{u}}) = 0, \tag{1}$$

$$\rho_f \left[\frac{\partial \varepsilon \bar{\boldsymbol{u}}}{\partial t} + \nabla \bullet \left(\varepsilon \bar{\boldsymbol{u}} \bar{\boldsymbol{u}} \right) \right] = -\varepsilon \nabla p + \varepsilon \nabla \bullet \mu_{eff} \nabla \bar{\boldsymbol{u}} + \boldsymbol{f}_p + \varepsilon \rho_f \boldsymbol{g}, \tag{2}$$

where ε is the local porosity, ρ_f is the fluid mass density, p is the coolant pressure, $\bar{\boldsymbol{u}}$ is the ensemble-averaged fluid velocity, $\boldsymbol{f}_p$ is the force density that pebbles exert onto the coolant and g is the gravitational acceleration. μ_{eff} is the effective viscosity which considered the effect of the turbulence onto the fluid boundary layer [18]. Because in the current FHR conceptual design the Reynolds number ($\mathrm{Re} = \frac{\rho_f u_0 d}{\mu_f}$, where d is the diameter of the pebble, u_0 is the superficial velocity of the coolant, and μ_f is the molecular viscosity of the coolant.) is typically within 100~1,000 [7], the Ergun drag model is adopted for the momentum source term, which can be written as [21]:

$$\boldsymbol{f}_p = -\beta \bar{\boldsymbol{u}}, \tag{3}$$

with $\beta(\varepsilon) = \frac{150(1-\varepsilon)^2 \mu_f}{\varepsilon d^2} + 1.75 \frac{\rho |\bar{\boldsymbol{u}}| (1-\varepsilon)}{d}$. For PB-FHR case, since coarse mesh (~2 times of the pebble diameter) is used for ensemble averaging, even in the boundary layer the viscous term is much smaller than the momentum source term $\boldsymbol{f}_p$, and in practice can be neglected for PBR coolant flow modeling [7, 22].

The ensemble-averaged energy balance equations for fluid phase can be written as [23, 24]:

$$\frac{\partial \varepsilon \rho_f c_{pf} T_f}{\partial t} + \nabla \bullet (\varepsilon \rho_f \bar{\boldsymbol{u}} c_{pf} T_f) = \nabla \bullet (\varepsilon k_f \nabla T_f) + h_{\mathrm{fs}} (T_f - T_s), \tag{4}$$

where T_{f} denotes cell-averaged fluid temperature, T_s is the pebble surface temperature, c_{pf} is the constant pressure specific heat of fluid, k_f is the fluid conductivity which is assumed to be constant in the PB-FHR case. h_{fs} is the heat transfer coefficient, which can be written as [24]:

$$h_{fs} = \frac{6(1-\varepsilon)}{d_{\mathrm{p}}} k_f Nu, \tag{5}$$

where the $\dfrac{6(1-\varepsilon)}{d_{\mathrm{p}}}$ term takes the packed pebble bed, pebble's spherical shape and diameter (d_{p}) into account [24] . The Nusselt number (Nu) model is based on the correlation function of the Reynolds number and Prandtl number (Pr) from Wakao model [25].

$$Nu = 2 + 1.1\mathrm{Pr}^{1/3}\,\mathrm{Re}^{0.6}\,. \tag{6}$$

Finite difference method with staggered grids is used for the discretization of the mass, momentum, and energy conservation equations. These discretized equations can be readily solved with any existing pressure-based solver. For PB-FHR case, the pressure-based solver is more appropriate compared with density-based solver as there is essentially no density variation throughout the core. Implicit solution scheme for the diffusion term and explicit scheme for the conduction/source term are adopted here. The solution of the fluid dynamics and heat transfer is given by using an in-house research code PEBble Fluid Dynamics (PEBFD) [20].

2.2. Pebble Flow Simulation Model with Thermal Heat Transfer

For the solid phase, the motion and rotation for each pebble can be written as:

$$m\frac{d\mathbf{v}_{\mathrm{i}}}{dt} = \boldsymbol{F}_{\mathrm{i}} = \sum_{\substack{j\neq i\\ j=1}}^{N} \boldsymbol{F}_{\mathrm{ij}} + \boldsymbol{W}_{\mathrm{i}} + m_{\mathrm{i}}\boldsymbol{g} + \boldsymbol{F}_{\mathrm{f,i}}, \tag{7}$$

$$J_{\mathrm{i}}\frac{d\boldsymbol{\omega}_{\mathrm{i}}}{dt} = \boldsymbol{M}_{\mathrm{i}}, \tag{8}$$

where $\mathbf{v}_{\mathrm{i}}$ is the velocity of the i$^{\mathrm{th}}$ pebble, $\boldsymbol{F}_{\mathrm{i}}$ is the net force on the i$^{\mathrm{th}}$ pebble including $\boldsymbol{F}_{\mathrm{ij}}$ the contact force from the j$^{\mathrm{th}}$ pebble, $\boldsymbol{W}_{\mathrm{i}}$ the wall contact force, $m_{\mathrm{i}}\boldsymbol{g}$ the gravitational force, and $\boldsymbol{F}_{\mathrm{f,i}}$ the fluid force which will be discussed in detail later. The pebble-pebble contact force $\boldsymbol{F}_{\mathrm{ij}}$, is composed of normal contact force $\boldsymbol{F}_{\mathrm{n,ij}}$ which is along the direction of $\boldsymbol{n}_{\mathrm{ij}}$（from the center of pebble j to the center of pebble i) and tangential contact force $\boldsymbol{F}_{\mathrm{t,ij}}$ which is along the plane perpendicular to $\boldsymbol{n}_{\mathrm{ij}}$. $\boldsymbol{M}_{\mathrm{i}}=-r_{\mathrm{i}}\boldsymbol{n}_{\mathrm{ij}}\times\boldsymbol{F}_{\mathrm{t,ij}}$ is the torque on i$^{\mathrm{th}}$ pebble due to the tangential components of contact forces, where r_{i} is the radius of i$^{\mathrm{th}}$ pebble. J_{i} is the momentum of inertial, and $\boldsymbol{\omega}_{\mathrm{i}}$ is the angular velocity.

Any numerical integration scheme is viable to solve above initial value problem, given the key pebble-fluid interaction forces from the fluid solver. In practice, we adopt a combined predictor-corrector approach to improve the overall integration efficiency [20].

In this work, the heat transfer of the solid phase is modeled at the same length scale for the fluid phase, i.e., the pebble thermal quantities (temperature, thermal conductivity) are averaged within each fluid cell. Hence we can use ensemble-averaged pebble flow energy balance model [23]:

$$\frac{\partial(1-\varepsilon)\rho_s c_{ps} T_s}{\partial t} = \nabla\bullet\left[(1-\varepsilon)k_{eff}\nabla T_s\right] + h_{\mathrm{fs}}(T_s - T_f) + q, \tag{9}$$

where ρ_s is the pebble density, c_{ps} is the specific heat of the pebble, T_s is the pebble surface temperature, k_{eff} is the effective pebble heat conduction coefficient which is assumed to be dependent on T_s based on

Zehner-Schlunder irradiated model [24], q is the fission heat source term. Although in PB-FHR, the conductive heat transfer among pebbles is very small, the effective conductivity k_{eff} takes other effect (such as radiative heat transfer) into account. Since we do not consider the neutronic effect, the fission reaction power distribution is assumed to follow a cosine law along the axial direction and constant along the radial direction based on existing HTR-10 and PB-FHR work [9, 21]. For each time step of CFD, the porosity and pebble velocities from the DEM calculation are used to calculate the drag force using Eq. (3). As mentioned at the beginning of this section, since the pebble flow properties evolve at a much slower rate than the coolant flow, the DEM solver and the CFD/thermal solver exchange data for every 1000 DEM steps as the default coupling frequency, with porosity and fluid properties invariant between data exchanging. Similar to the fluid solver, the solid heat transfer equation is solved by explicitly solving the nonlinear term and implicitly solving the diffusion term.

3. MECHANICAL-THERMAL ANALYSIS OF A SMALL-SCALE PB-FHR

In this section, we study the mechanical-thermal behavior in the PB-FHR design, where the coolant density is greater than the pebble density and the fluid-pebble interaction is strong compared with the net body force $(\rho_f V_S - m)g$. Currently, there is no matured design configuration for PB-FHR with practical operation. For better comparison, we use the same core geometry as the HTR-10 design except making it upside down. PB-FHR pebble flow operation condition is applied. Two cases are studied in this work. In the first case, the mass flow rate of the fluoride salt coolant is 198.5 kg/s and the pebble Reynolds number is Re=468 And for the second case, the mass flow rate is a quarter of the first case's (which is 49.625 kg/s) and the corresponding pebble Reynolds number is Re=117.

3.1. Geometry, Design Parameters and Simulation Setup

Same geometry dimensions and total pebble number (30,000) as used in the HTR-10 configuration are used for the PB-FHR case (inlet is at the bottom). The side view of the reactor geometry is shown in Fig. 1, with the z=-60 cm at the outlet. The physical parameters for the pebble and coolant are listed in Table I. The thermal conductivity for the graphite is determined based on Zehner-Schlunder irradiated model, which is around 0.08 W/cm/K at 800K-900K. For the molten salt coolant, the thermal conductivity for Flibe is used. Since the coolant is nearly incompressible and the inlet-outlet temperature difference is much smaller in PB-FHR compared with the gas-cooled counterpart, the coolant property is assumed to be constant during operation. The inlet temperature for the coolant is assumed to be 773 K (500 C). The cylindrical core has a height of 1.8 m and diameter of 1.8 m. The radial resolution is dr=11.25 cm and the axial resolution is dz=14.4 cm. The graphite wall thickness is assumed to be 1 m and the ambient temperature is assumed to be the same as the coolant temperature (773K). The neutronic power distribution is assumed to follow a cosine law along the axial direction as shown in Fig.2, which is equivalent to a total of 20 MWt power within the cylinder core. For the pebble friction coefficient, in reality it is temperature dependent [26]. However, for the studied small-scale FHR case, since the temperature variation is very small within the core, we assume a uniform μ=0.2 which does not change with the temperature, although a temperature-dependent friction coefficient is quite necessary for the large-scale PBR case where the temperature variation is significant within the core. Other quantities such as the thermal conductivity and specific heat are also assumed to be temperature independent in this work.

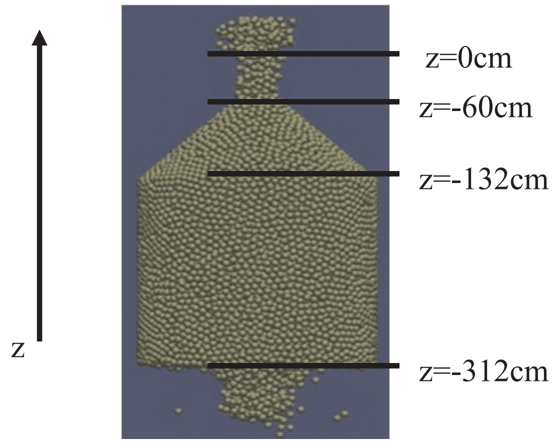


Figure 1. Reactor geometry

Table I. Pebble and coolant physical properties for PB-FHR simulation

Pebble	Radius	Mass	Young's modulus	k_n/k_t
	3 cm	210 g	1E9 Pa	7/2 *
	Poisson ratio	Specific heat	Friction coefficient	Thermal conductivity
	0.3	1.8E3 J/kg·K	0.2	8 W/m/K
Coolant	Density	Molecular viscosity	Specific heat	Mass flow rate (2 cases)
	1950 kg/m^3	1E-2 Pa·s	2.4E3 J/kg·K	198.5 and 49.625 kg/s
	Inlet temperature	Outlet pressure	Thermal conductivity	Melting temperature
	773 K	constant	1 W/m/K	732 K

* [13].

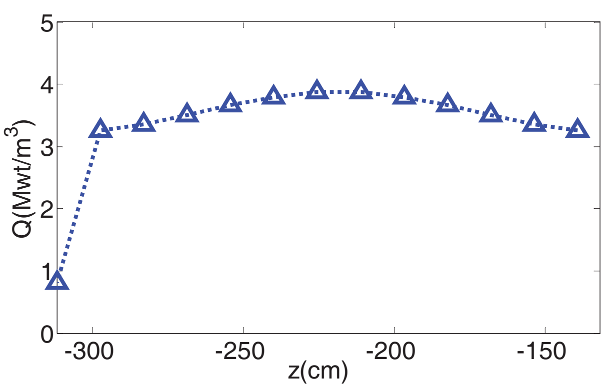
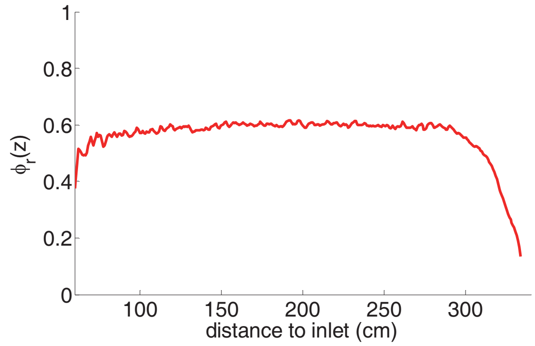


Figure 2. In-core neutronic power distribution

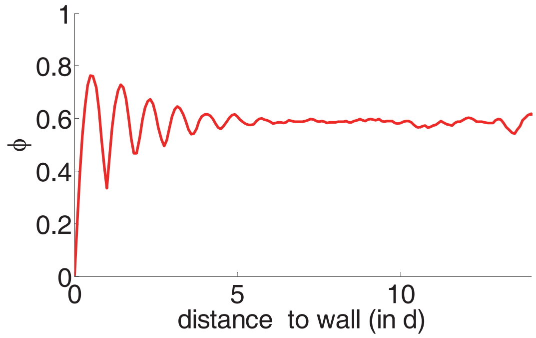
3.2. Mechanical and Thermal Predictions in the PB-FHR Core

The larger PB-FHR design with the correspondingly higher mass flow rate is studied first (case 1). Due to the finite size geometry, there will be visible variations of pebble volume packing fraction or the coolant porosity along both the radial direction and axial direction, which are shown in Fig. 3 for case 1. In Fig.

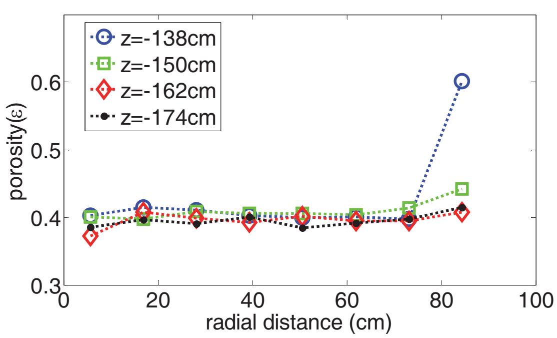
3(a-b), the mesh size is set as dr=dz=0.5 cm in order to capture the radial oscillation. Although in practice a much coarser grid system is used for the fluid-thermal modeling (solutions of the mass, momentum, and energy conservation equations), this boundary effect is still observable as shown in the Fig. 3(c-d). We can see that the porosity is higher in the near wall region than the inner region, which causes a higher flow velocity in the near wall region (channeling effect or by-pass effect, as shown in Fig.4). As indicated in previous work [20], the fluid-pebble interaction can appreciably affect the porosity distribution compared with pebble flow only simulation and it is very important to use a coupled fluid-pebble flow model in order to precisely capture the porosity profile.



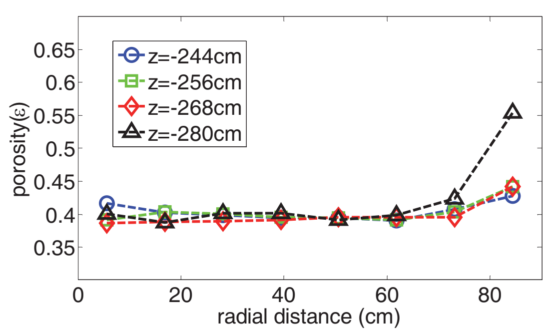
(a) axial distribution (on fine meshes)



(b) radial distribution (on fine meshes)



(c) upper core (on coarse meshes)



(d) lower core (on coarse meshes)

Figure 3. Porosity distribution at different heights (case 1)

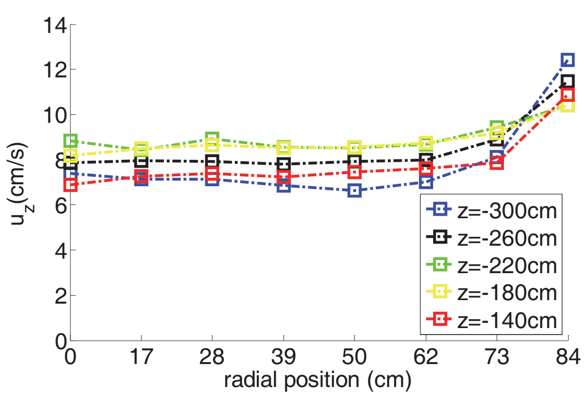
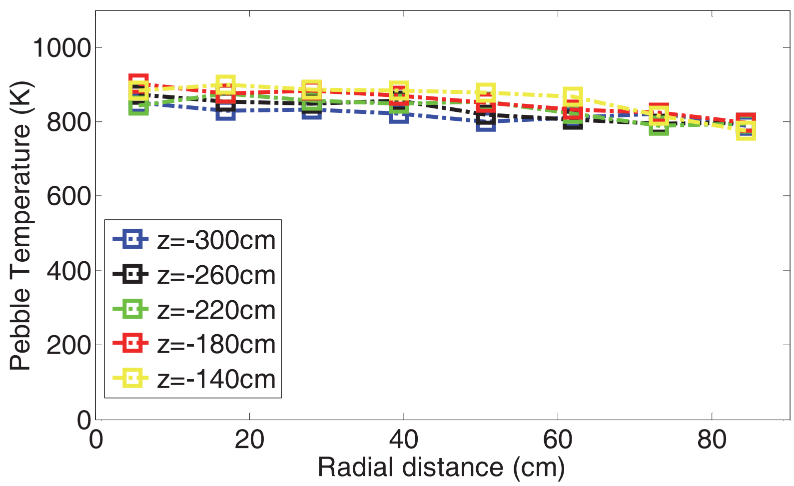
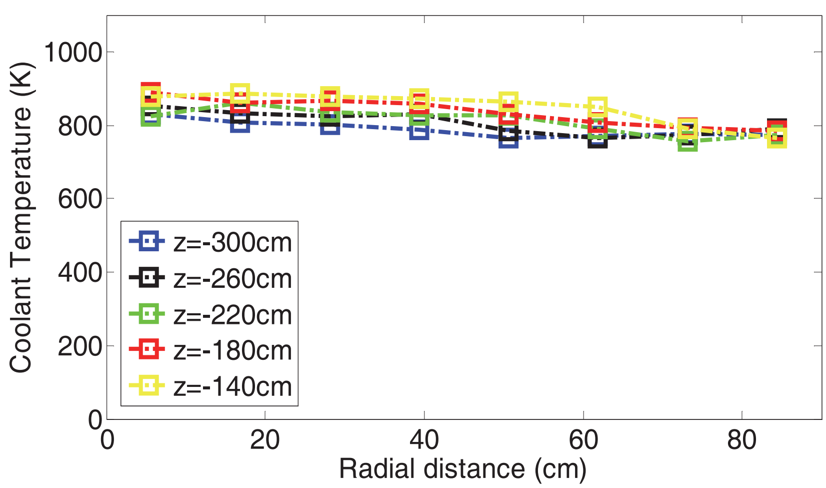


Figure 4. Axial fluid velocity profile at different heights (case 1)

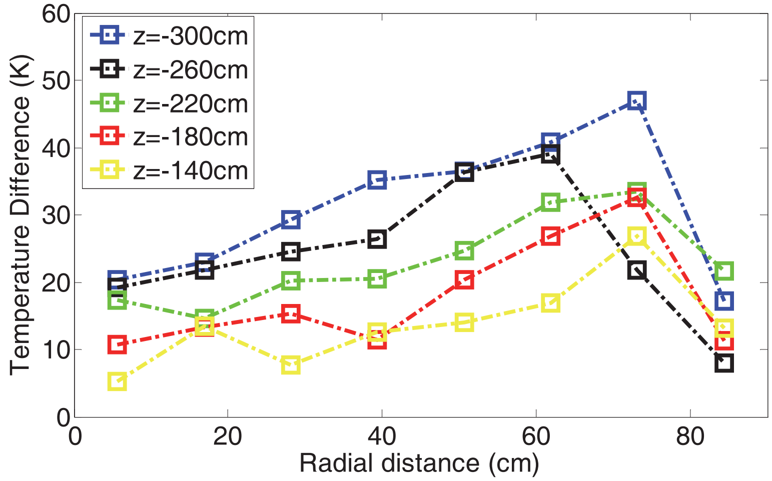
The higher coolant velocity in the near wall region will enhance local heat transfer and brings fission heat out more efficiently, and consequently result in a lower near wall fuel temperature, as shown in Fig. 5a, which indicates a very slight temperature change along the axial direction. For the given 773 K inlet temperature, the average outlet pebble surface temperature is around 900 K (Fig. 5a). Fig. 5a and b also suggests that, with the power density twice as large as the HTR-10 design, the temperature difference between inlet and outlet for FHR is much smaller than the HTR-10 [8, 10] due to the much higher density and thus mass flow rate of the molten salt coolant. The distribution of T_s-T_f is shown in Fig. 5c, which also suggests a very small temperature difference between the fluid and solid phase throughout the core. As a comparison, we studied case 2 which has only 1/4 of the mass flow rate as case 1, and the cell-averaged fluid temperature, pebble temperature, fluid-solid temperature difference and axial velocity distribution are shown in Fig. 6. From the figure we can see that the pebble temperature is higher than case 1's with reduced coolant mass flow rate. And by reducing the mass flow rate to a quarter of the case 1, the coolant can still effectively carry the fission heat out of the core effectively, giving this design a large safety margin in case of a LOFC accident. As for the axial coolant velocity, the reduction in the mass flow rate will not significantly change the overall radial profile of u_z (normalized), which is mainly determined by the porosity radial distribution.



(a) pebble surface temperature distribution

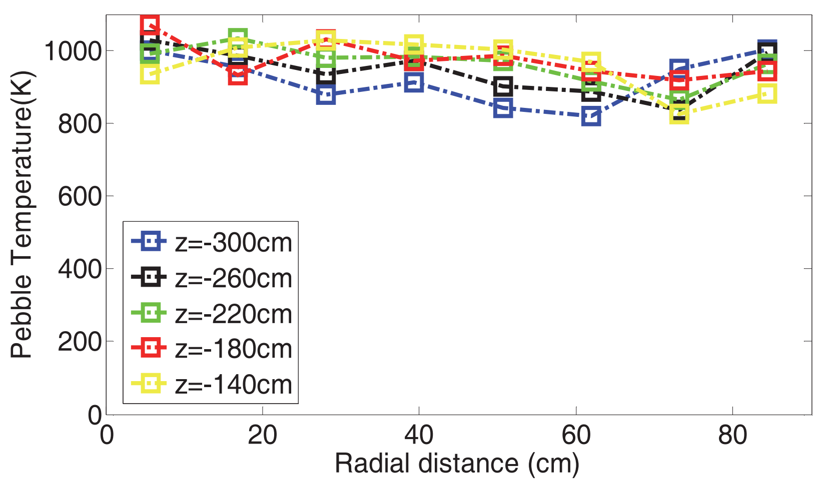


(b) coolant temperature profile

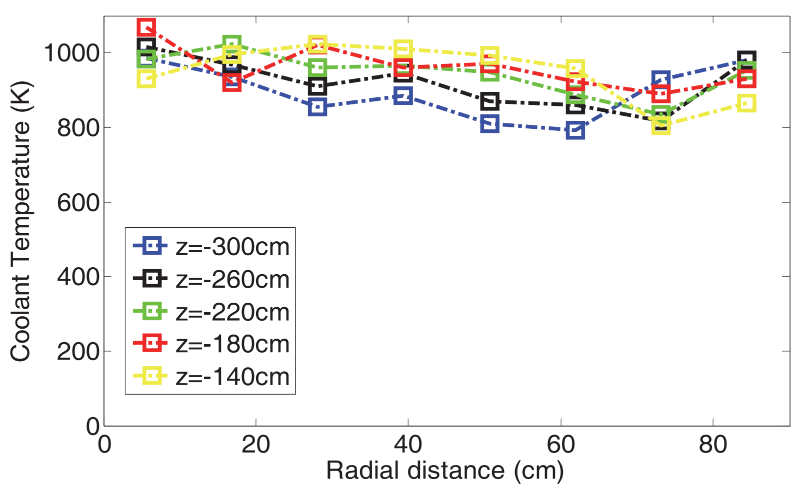


(c) temperature difference distribution

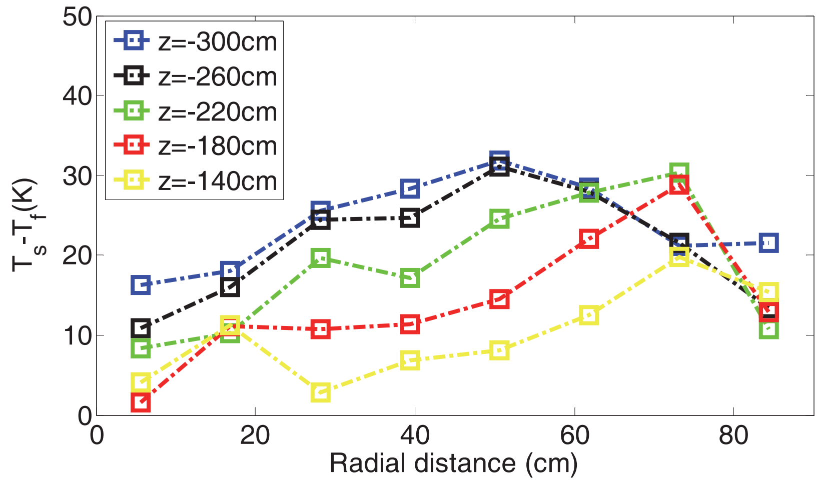
Figure 5. Cell-averaged fuel and coolant temperature profile (Re=468)



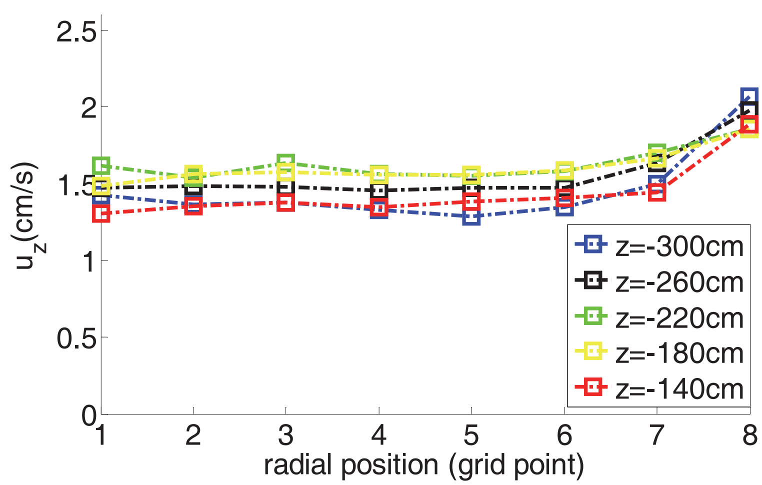
(a) pebble surface temperature distribution



(b) coolant temperature profile



(c) temperature difference distribution



(d) radial distribution of fluid axial velocity

Figure 6. Cell-averaged fuel and coolant temperature profile (Re=117)

4. CONCLUSIONS

Based on the coupled DEM and CFD methodology in previous PBR design simulations [15], a multi-physics thermal-fluids model accounting for the pebble motion, fluid motion and heat transfer are presented in this work and are applied to PB-FHR design analysis. The new coupled model is resolved by a hybrid DEM-CFD solution scheme using semi-implicit finite differencing approach. Results suggest that in a pebble bed design, the finite-sized wall will cause a high porosity region near the boundary and significantly affect the fluid-thermal behavior. Since the fluid-pebble momentum interaction can greatly affect the near wall porosity distribution, and the pebble flow mechanical behavior is heavily dependent on the pebble surface friction coefficient which is temperature dependent, it is necessary to adopt such a fully coupled model to accurately model the multi-physics phenomena within a large-scale PB-FHR system. Although for a small-scale, molten-salt cooled PBR, this temperature dependence is not prominent, a transient, fully coupled mechanical-thermal model is still needed as it can be further applied to off-normal scenario analysis and can be extended to large-scale, gas-cooled PBR applications. Also, due to the high density of the molten salt coolant, the coolant temperature has much smaller variation along the axial direction than the gas-cooled case, and the pebble Reynolds number is also much smaller (Re=117 for case 2 versus ~2E3 in HTR-10). Therefore this feature of the PB-FHR design allows a much higher fission power density within the core compared with HTR-10 design, without the requirement for the pressure vessel to operate under high pressure.

Future work will be focused on two areas, first is a study of the gas-cooled PBR case, in which a compressible fluid solver needs to be adopted to account for the forced convection of coolant gas within the core. The second effort will be made towards the discrete modeling of the pebble heat conduction instead of current cell-averaged model, so that the radial temperature distribution within a pebble can be well accounted for which is essential for accurate neutronic calculation and coupled neutronic-thermal modeling.

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