A High-Fidelity Multiphysics Computational Model for Pebble Bed Gas Reactor based on Open-Source Software

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INTRODUCTION

The high temperature pebble bed reactor (HT-PBR) is emerging as a next generation nuclear reactor technology owing to its high thermal efficiency and inherent safety features [1]. A typical HT-PBR is fueled with hundreds of thousands of pebbles piling up within the reactor vessel as shown in Fig. 1. A fuel pebble is effectively a spherical ball of ~6 cm diameter, filled with tens of thousands of TRISO (TRi-structural ISOtropic) particles (see Fig.1). The TRISO particle is prestigious for its ability to withstand high temperatures and prevent the release of radioactive fission products [2]. One distinguishing feature of the HT-PBR design from traditional reactors is that the fuel elements are not stationary. Instead, the pebbles continuously circulate through the reactor core throughout the plant's operational lifespan [3]. During each circulation cycle, the fuel content within the pebbles will be carefully evaluated based on its condition to determine whether the pebble is either reinserted into the reactor or removed from it. As a result, it is important to note that the deviation in the fuel content occurring in each pebble is due to changes in the speed, position, and circulation path.

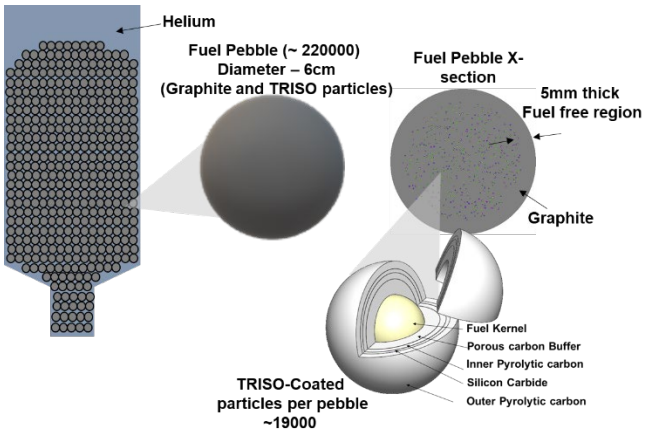

Fig. 1. Depicts the schematic overview of HT-PBR.

Reactor analysis tools based on either deterministic or probabilistic (Monte Carlo) methods have been used to simulate the neutronic physics in the HT-PBR. In the deterministic method, the radiation transport equation is numerically solved by discretizing and meshing the domain. In the Monte Carlo method, the transport problem is solved by tracking and simulating the particle histories. However, the deterministic method faces disadvantages when simulating complex geometries such as those present in the HT-PBR. Conversely, Monte Carlo based computational tools on the other hand can solve three-dimensional transport problems with complicated geometries [4].

Various Monte Carlo-based particle transport codes including MCNP, Serpent, and OpenMC are readily available for use in performing HT-PBR analysis. Among these, OpenMC code is a relatively recent but unique addition, characterized by its open-source nature, inherent high-performance capabilities, and user-friendly interface. Therefore, it was decided to use OpenMC for neutronics analysis in this work.

Multiphysics modeling and simulation of a full-scale HT-PBR reactor model is a challenging task. A report for modeling the fully coupled neutronic thermal hydraulic HT-PBR plant has been recently published by Idaho National Laboratory (INL) regarding to one Nuclear Regulatory Commission project [5]. The INL work essentially develops a Multiphysics Object Oriented Simulation Environment (MOOSE) based interface that integrates Griffin (neutronics), Pronghorn (thermal-hydraulics), and BISON (fuel performance) applications. This simulation considered a critical assumption, characterizing the core region as simple and axis-symmetric in a two-dimensional manner. Uniform pebble velocity and homogenous porosity distribution was assumed. It is crucial to note that the pebble velocity during each pass is contingent on its position within the core, and the spatial dependency of neutron flux further concentration creates further complications.

The pebbles flow in the reactor core relate to the particulate flow. Over the past two decades, various strategies have been developed to numerically describe particulate flows, which are prevalent in both natural and industrial settings. In this context, two main approaches for modeling the particulate phase have emerged: the continuum approach and the discrete approach [6, 7]. Unlike the continuum approach, the discrete approach does not rely on continuum mechanics to describe particulate flow. Instead, it focuses on individually modeling the motion of each particle, considering specific treatments for particle collisions [6, 7].

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In this work, the primary aim is to propose a Multiphysics coupling scheme that utilizes the open-source software CFDEM and OpenMC for analyszing the full-scale HT-PBR reactor core. The Discrete Element Method (DEM) was employed to investigate both the movement of pebbles and the porosity within the Pebble Bed Reactor (PBR) model. The pebbles are primarily influenced by the drag force resulting from fluid-particle interactions. To simulate the fluid motion within the PBR, the Navier-Stokes equation and the continuity equation that govern the physics phenomena are coupled and solved using the OpenFOAM software. Consequently, a Computational Fluid Dynamics-Discrete Element Method (CFD-DEM) scheme has been established and implemented by utilizing the open-source CFDEM software to consider the interactions between the fluid and particles in the system.

METHODOLOGY

In the open source CFDEM coupling software, the solver, cfdemSolverPiso is coupled to PisoFOAM with the DEM code LIGGGHTS. PisoFOAM is a finite volume-based solver in OpenFOAM 5.0, for solving incompressible, turbulent flow with PISO algorithm [8]. In cfdemSolverPiso, the volume averaged Navier-Stokes equations are solved including the momentum exchange and motion of discrete particles (mimicking pebbles in HT-PBR) whose trajectories are computed in LIGGGHTS. Following the brief overview of cfdemSolverPiso to model the different solid interaction forces, fluid flow through the porous media, and momentum exchange between fluid and pebble are described.

The DEM employs a Lagrangian approach that involves the explicit tracking of trajectories for all particles within the computational domain by solving the linear and angular momentum equations described by Eq.(1).

$$\begin{aligned} m_i \frac{d\boldsymbol{U}_i}{dt} &= \sum_{j=1}^{n_j^c} \boldsymbol{F}_{i,j}^c + \boldsymbol{F}_i^g + \left(\boldsymbol{F}_i^b + \boldsymbol{F}_i^d\right)_f + \boldsymbol{F}_i^a \\ I_i \frac{d\boldsymbol{\omega}_i}{dt} &= \sum_{j=1}^{n_j^c} \boldsymbol{M}_{i,j}^{\boldsymbol{c}} \end{aligned} \quad , \qquad (1)$$

where $\boldsymbol{U}_i$ and $\boldsymbol{\omega}_i$ are the translational and rotational velocity of i^{th} particle, respectively. The contact force $\boldsymbol{F}_{i,j}^{\boldsymbol{c}}$ and torque $\boldsymbol{M}_{\boldsymbol{i,j}}^{\boldsymbol{c}}$ act on the i^{th} particle due to interaction with other particles (j) or walls. The term n_j^c represents the total number of contacts of particle i. $\boldsymbol{F}_i^{\boldsymbol{g}}$ is the gravitational force. $\boldsymbol{F}_i^b$ and $\boldsymbol{F}_i^d$ are the buoyancy force and drag force from interactions with the surrounding fluid. Additional forces including van der Waals, electrostatic, magnetic, cohesiveness, or any external forces are collectively represented by the force component $\boldsymbol{F}_i^a$. In this study, the dominant forces considered are particle-particle interactions, particle-wall interactions, gravitational, buoyancy, and drag forces.

In the Computational Fluid Dynamics (CFD) method, the continuous fluid domain is divided into discrete cells for numerical analysis. By solving the continuity equation and locally averaged Navier-Stokes equations shown in Eq. (2) and (3), the locally averaged quantities such as velocity, pressure, and density can be determined. To perform CFD simulations in the CFDEM software, it is coupled with OpenFOAM 5.0, an open-source software based on the finite volume method (FVM). OpenFOAM utilizes FVM for discretizing and solving the governing equations of fluid flow.

$$\frac{\partial \varepsilon \rho_f}{\partial t} + \nabla \cdot \left(\varepsilon \rho_f \boldsymbol{u}\right) = 0 \quad , \qquad (2)$$

$$\begin{aligned} \frac{\partial \varepsilon \rho_f \boldsymbol{u}}{\partial t} + \nabla \cdot \left(\varepsilon \rho_f \boldsymbol{u}\boldsymbol{u}\right) - \varepsilon \nabla \cdot \left(\mu \nabla \boldsymbol{u}\right) \\ = -\nabla p - \boldsymbol{F}^{pf} + \varepsilon \rho_f \boldsymbol{g} \end{aligned} \quad . \qquad (3)$$

In the equations, ρ and μ are the fluid density and viscosity, respectively. The variables $\boldsymbol{u}$ and p represent the fluid velocity and pressure fields, respectively. The void fraction (ε) is defined as $\varepsilon = 1 - v_p/v_c$, where v_p is the volume occupied by the particles and v_c is the total volume of the cells. The momentum exchange between the particles and the fluid, denoted as $\boldsymbol{F}^{pf}$, is modelled using the Ergun equation, which is an empirical correlation established by Zeki Ergun in 1952 to predict a pressure drop or pressure loss in packed and fluidized beds [6].

The OpenMC package includes a built-in class called openmc.deplete() that assesses material decay and transmutation through numerical integration methods by solving the Bateman equation as follows

$$\frac{dN_i(t)}{dt} = \lambda_{i-1} N_{i-1}(t) - \lambda_i N_i(t) \quad , \qquad (4)$$

where N_i is the i^{th} nuclide concentration and λ_i is the decay coefficient of the material. The decay and transmutation of the nuclides contributes to the heat energy within the pebble. This heat increases the reactor's internal temperature, impacting the material cross sections. Further, this energy is carried through the helium gas flow through the porous structure of the PBR. Therefore, to numerically model the heat energy interactions within the PBR reactor, the energy conservation equation in fluid and solids (pebbles) and the above momentum equation are also solved. The fluid and solid heat energy conservation [5, 9] is described in Eqs.(5) and (6), respectively.

$$\begin{aligned} \varepsilon \rho_f C_{p,f} \frac{\partial T_f}{\partial t} + \varepsilon \rho_f C_{p,f} \nabla \boldsymbol{u} \cdot (\mathrm{T}_f) - \nabla \cdot (\varepsilon k_f \nabla \mathrm{T}_f) \\ + \alpha \left(T_f - T_s\right) = \dot{q}_f''' \end{aligned} \quad , \qquad (5)$$

$$\left(1-\varepsilon\right) \rho_s C_{p,s} \frac{\partial T_s}{\partial t} - \nabla \cdot (\varepsilon k_s' \nabla \mathrm{T}_s) + \alpha \left(T_s - T_f\right) = \dot{q}_s''' \quad . \qquad (6)$$

These equations are coupled by the heat transfer coefficient (α) and solved simultaneously. In solid (pebbles), the heat source $\dot{q}_s'''$ counts the heat generated from the fuel. The average fuel pebble temperature (T_s) is computed considering spherically symmetric one-dimensional subscale heat conduction models in each pebble-bed mesh element.

Precise modeling of the energy and heat conduction equation relies significantly on the thermal conductivities of the fluid and solid (k_f and k_s). Ensuring accuracy in these properties is crucial for assessing the temperature distribution within the reactor. In fluid flow through porous media, the *effective* thermal conductivity (k_f') is used instead contingent upon the Reynolds and Prandtl numbers. The correlation used for k_f' is developed based on the Peclet number (Pe), which is the ratio of Reynolds to Prandtl numbers, and shown in Eq. (7)

$$k_f' = \varepsilon k_f + C_0 \mathrm{Pe} k_f \quad , \tag{7}$$

where C_0 is a constant coefficient to be determined. Likewise, acquiring the *effective* conductivity (k_s') in the solid region as outlined in Eq. (6) is more intricate. Various effective thermal conductivity models for solid pebbles are available in the literature [10–12]. In this work, the Zehner-Bauer-Schlünder (ZBS) model is considered, incorporating all heat transfer modes. In the context of the numerous interaction modes between pebbles that contribute to this conductivity, surpassing even the modes observed in fluid flow across pebbles. These modes involve radiation between pebbles, direct conduction at contact points, and pebble-conducted heat through the fluid present between pebbles. As such, the effective thermal conductivity of the solid encompasses these varied interaction modes. It is worth noting that the International Atomic Energy Agency recommends the utilization of the ZBS effective thermal conductivity model in pebble bed reactors [13]. For brevity, we refer the thermal conductivity model is referred to [10-12].

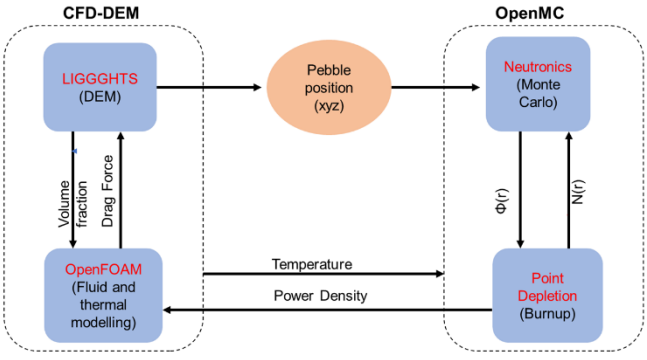

Fig. 2. Depicts the block diagram and coupling mechanisms between OpenMC and CFD-DEM.

In the *cfdemSolverPiso,* Thermal modeling is not included in cfdemSolverPiso. Therefore, we will include thermal modeling is not included. Therefore, thermal modelling will be included and verified with the existing test cases. and verify it with the existing test cases. The coupling between CFDEM and OpenMC is depicted in the block diagram shown in Fig. 2. CFDEM generates a more realistic representation of pebble positions within the PBR for OpenMC. OpenMC, in turn, analyzes the neutronic behavior and depletion of the nuclides. Additionally, the thermal model incorporates the heating source resulting from depletion and calculates the temperature distribution within the reactor. This crucial temperature distribution influences the neutronic calculations performed by OpenMC.

CASE STUDY & PRELIMINARY RESULT

This work adopts the X-energy's Xe-100 core design [1] as the case study to test the computational methodology. The Xe-100 core has a hopper-like shape with a maximum diameter of 2.4 meters and a minimum diameter of chute 0.52 meters (see Fig. 3). In the original Xe-100 design, the active core's height is approximately 11 meters, accommodating over 200,000 pebbles. Fuel pebbles are introduced at the top of the core with an assumed velocity of 5 m/s. The geometric properties and composition of each pebble are taken as the same of Xe-100 design [1]. The outlet from the chute is considered closed during loading, and the core is filled within an assumed time of 105 seconds out of a total of 220,848 pebbles. A settling time of 10 seconds is further allocated. The DEM code incorporates pebble-wall and pebble-pebble interactions, rolling friction, and gravitational forces. The position of each pebble is generated by DEM code and then exported to OpenMC using a Python script. A thick graphite layer (~1.24 m) is modeled surrounding the core (diameter ~4.88 m) in OpenMC. A vacuum boundary condition is considered surrounding the graphite layer. Considering their minor effect in gas cooled reactor, the top and bottom leakages are neglected in the current model by imposing mirror reflective boundary conditions. The lattice of 10×10×10 is generated in each pebble and the whole core (see Fig. 4). The lattice creation feature in OpenMC has the advantage of reducing the time consumption of simulation significantly [2]. This approach generates the virtual lattice in the physical model and maps the position of TRISO's to specific lattice positions, thereby reducing the required search space [2]. The OpenMC code is executed in the VCU Oak HPC with 40 processors for the steady-state simulation of the core. The value of the effective neutron multiplication factor (k_{eff}) and leakage fraction resulting from the calculation are summarized in Table I.

Table I. Steady-state whole core calculation result.

k_{eff}	Leakage fraction (%)	Simulation time
1.39160 +/- 0.00021	4.780 +/- 0.005	3 hours

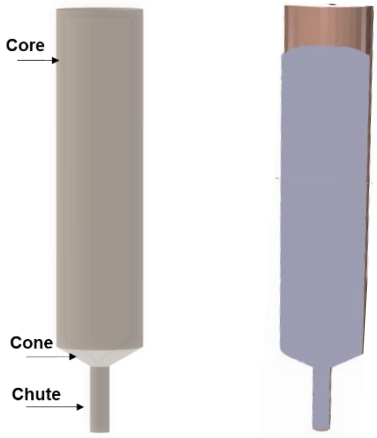

Fig. 3. Depicts the CAD model of PBR reactor core (left) and the core loaded with the pebbles (right).

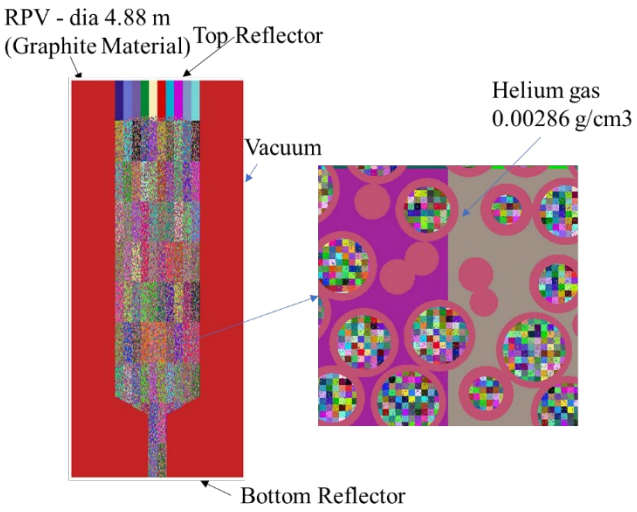

Fig. 4. Depicts the lattice configuration in the reactor core (left) and the fuel pebble (right).

CONCLUSIONS

This paper provides a detailed description of a high-fidelity Multiphysics analysis of a HT-PBR core utilizing a computational coupling scheme established by open-source software CFD-DEM and OpenMC. The positions of the moving pebbles are determined using the DEM based LIGGGHTS code and loaded into OpenMC, which performs the subsequent steady-state neutronics calculations. The work reports the steady-state neutronics operation results for an operational HT-PBR core based on the Xe-100 design, which contains more than 200,000 pebbles. Burnup and additional dynamics analysis of the HT-PBR performance will be continued with the established open-source computational model.

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