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A SIMPLIFIED DEM-CFD APPROACH FOR PEBBLE BED REACTOR SIMULATIONS

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ABSTRACT

In pebble bed reactors (PBR's), the pebble flow and the coolant flow are coupled with each other through coolant-pebble interactions. Approaches with different fidelities have been proposed to simulate similar phenomena. Coupled Discrete Element Method-Computational Fluid Dynamics (DEM-CFD) approaches are widely studied and applied in these problems due to its good balance between efficiency and accuracy. In this work, based on the symmetry of the PBR geometry, a simplified 3D-DEM/2D-CFD approach is proposed to speed up the DEM-CFD simulation without significant loss of accuracy. Pebble flow is simulated by a full 3-D DEM, while the coolant flow field is calculated with a 2-D CFD simulation by averaging variables along the annular direction in the cylindrical geometry. Results show that this simplification can greatly enhance the efficiency for cylindrical core, which enables further inclusion of other physics such as thermal and neutronic effect in the multi-physics simulations for PBR's.

Key Words: Pebble Bed Reactors, Discrete Element Method, Computational Fluid Dynamics, Multi-physics Coupling

1. INTRODUCTION

As a promising candidate for the next generation nuclear reactor system, Pebble Bed Reactors (PBR's) have great advantages in fuel efficiency and operation safety [1]. High-accuracy modeling of pebble flow in PBR's can provide reliable evaluation for the reactor's neutronic performance, thermal-hydraulic efficiency and safety threshold. Besides accuracy, simulation efficiency is also important. Fast computation can enable long term performance evaluation, quick decision for reactor operators under accident conditions [2], and potential to account for more physics.

Pebble flow and coolant flow in a PBR can be considered as a dense time varying fluid-particle system, in which pebble flow is a discrete solid phase and coolant flow is a continuum phase. The pebble motion is governed by pebble gravity and interactions of pebble-pebble, pebble-wall and pebble-fluid. For the particulate phase modeling, high-precision deterministic discrete approach, represented by Discrete Element Method (DEM) [3], is widely adopted. DEM is based on Newton's law of motion and contact mechanics, which can accurately model the inter-particle physics such as repulsion and cohesion. Based on these high-fidelity models, consequent

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individual particle's motion can be calculated using explicit time integration. Very small time step length (~10μs) is usually adopted for graphite pebbles in order to preserve the contact physics [4]. Due to its high accuracy, DEM is widely used in modeling various particulate or granular systems [5], at the cost of intensive computation workload. For the fluid phase modeling, conventional Computational Fluid Dynamics (CFD) approaches which solve the continuum based local averaged Navier-Stokes equations [5], are generally applied because of its relatively good efficiency and code availability. Owing to its continuum-based nature, CFD approach usually adopts much larger time step length (>1ms) in time integration for macroscopic systems.

In view of the advantages of both DEM and CFD approaches, the coupled DEM-CFD strategy is popular to model the fluid-particle system [6-11], including the pebble flow and coolant flow in a PBR [11]. The DEM solver is able to calculate individual particle's motion and rotation, while the CFD solver uses a set of finite volume fluid cells which usually contain tens of particles, and calculate the averaged solid and fluid quantities within each cell. The two-way coupling between solid and fluid is realized by calculating and exchanging fluid-particle interaction force between DEM and CFD solvers. This coupling strategy can account for high-fidelity solid-solid interaction with moderate accuracy in fluid calculation and fluid-solid interaction.

Although DEM-CFD is a good choice for fluid-particle system simulation, it is still too expensive for PBR application. As there are tens of thousands of densely packed fuel pebbles within the active core, and the coolant speed is considerably high (the order of 100m/s), frequent coupling information exchange is necessary to maintain the accuracy which also leads to large computational workload. Since all proposed PBR schemes have axial-symmetrical geometry (either cylindrical or annular), a simplified 3D-DEM/2D-CFD approach is proposed in this work to simulate PBRs. The inter-particle physics is still modeled by the full 3D DEM approach, while the fluid quantities are averaged along the annular direction. Results show that this simplification can greatly enhance the computation efficiency, with insignificant loss on the overall accuracy.

2. MODEL DESCRIPTION

2.1. Governing Equations for Pebble Motion

The equations of motion for the pebbles are:

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

$$J_{\mathrm{i}}\frac{d\boldsymbol{\omega}_{\mathrm{i}}}{dt} = \boldsymbol{T}_{\mathrm{i}}\ , \tag{2}$$

where $\mathbf{v}_{\mathrm{i}}$ is the velocity of the *i*th pebble, $\boldsymbol{F}_{\mathrm{i}}$ is the net force on the *i*th pebble including $\boldsymbol{F}_{\mathrm{ij}}$ the contact force from the *j*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. $\boldsymbol{T}_{\mathrm{i}}$ is the torque on *i*th pebble due to the tangential components of contact forces, $\boldsymbol{J}_{\mathrm{i}}$ is the momentum of inertial and $\boldsymbol{\omega}_i$ is the angular velocity.

For pebble-to-pebble contact force $\boldsymbol{F}_{ij}$, it is composed of normal contact force $\boldsymbol{F}_{n,ij}$ and tangential contact force $\boldsymbol{F}_{t,ij}$. According to Hertzian contact mechanics [12], the normal contact force $\boldsymbol{F}_{n,ij}$ between two spheres i and j with radius r_i, r_j and velocity $\mathbf{v}_i$, $\mathbf{v}_j$, is given as:

$$\boldsymbol{F}_{n,ij} = \sqrt{\frac{r_i r_j}{r_i + r_j}}(k_n \delta_{ij}^{1.5} - \gamma_n \delta_{ij}^{0.5} v_{n,ij})\mathbf{n}_{ij}, \tag{3}$$

where k_n and γ_n are material elastic and visco-elastic constants respectively, $\mathbf{v}_{n,ij}$ is the relative normal velocity defined as $(\mathbf{v}_i - \mathbf{v}_j)\cdot\mathbf{n}_{ij}$, $\mathbf{n}_{ij}$ is the unit normal vector pointing from the center of pebble j to the center of pebble i, and δ_{ij} is the overlapping depth between two pebbles. For the tangential contact force, the stick-slip model [4, 12] is used combined with the Columb's dry friction law:

$$\boldsymbol{F}_{t,ij} = -k_t \delta_{ij}^{0.5} \int_{t_0}^{t} \mathbf{v}_{t,ij} dt, \quad \left\| \boldsymbol{F}_{t,ij} \right\| \le \mu \left\| \boldsymbol{F}_{n,ij} \right\| , \tag{4}$$

where k_t is the tangential elastic constant, and $\mathbf{v}_{t,ij}$ is the relative tangential velocity defined as :

$$\mathbf{v}_{t,ij} = \mathbf{v}_i - \mathbf{v}_j - \mathbf{v}_{n,ij} - (r_i \boldsymbol{\omega}_i \times \mathbf{n}_{ij} + r_j \boldsymbol{\omega}_j \times \mathbf{n}_{ij}) . \tag{5}$$

For the fluid-to-pebble force $\boldsymbol{F}_{f,i}$, it represents the forces that are exerted on the pebble from fluid, in the case of dense and slow moving granular flow, the major interaction force is the drag force and pressure gradient force, which can be expressed as

$$\boldsymbol{F}_{f,i} = \boldsymbol{F}_D + \boldsymbol{F}_P , \tag{6}$$

$$\boldsymbol{F}_D = \frac{1}{2}\rho(\boldsymbol{u} - \boldsymbol{u}_P)\left\|\boldsymbol{u} - \boldsymbol{u}_P\right\| C_d \pi r^2 \alpha(\varepsilon) , \tag{7}$$

$$\boldsymbol{F}_P = -\int_{V_P} \nabla p dV , \tag{8}$$

where $\boldsymbol{F}_D$ is the De Felice drag force [5], $\boldsymbol{F}_P$ is the pressure gradient force, $\boldsymbol{u}$ is the fluid velocity, p is the pressure, ρ is the coolant density, $\boldsymbol{u}_P$ is the pebble velocity, V_P is the volume of a pebble, ε is the local porosity, C_d is the drag coefficient, $\alpha(\varepsilon)$ is an empirical function determined by ε and the Reynolds number *Re* [5-8].

After obtaining the fluid-to-pebble force $\boldsymbol{F}_{f,i}$, the pebble-to-fluid force intensity $\boldsymbol{f}_P$, which is the force exerted onto a fluid cell from the pebbles within or overlap with this cell, can be calculated. [4, 5]. The expression of $\boldsymbol{f}_P$ is shown as in Eq.(9),

$$\boldsymbol{f}_P = -\sum_{i}^{N_c} (\beta_i \sum (\boldsymbol{F}_D + \boldsymbol{F}_P)) / V_{cell} , \tag{9}$$

where N_c is the number of pebbles within a fluid cell, V_{cell} is the volume of the fluid cell, and β_i is the volume fraction of i^{th} pebble that falls into the cell. The $\boldsymbol{f}_P$ term is constant within each fluid cell and will be used in the fluid calculation.

2.2. Governing Equations for Fluid Motion and the Coupling Strategy

For standard CFD modeling, the numerical solution for incompressible local averaged Navier-Stokes (N-S) equation is needed. The 2-D N-S equations for the fluid phase in the cylindrical system are (constant coolant density is assumed):

$$\frac{\partial(\varepsilon)}{\partial t}+\frac{1}{r}\frac{\partial(\varepsilon r u_r)}{\partial r}+\frac{\partial(\varepsilon u_z)}{\partial z}=0\,, \tag{10}$$

$$\rho_f\left(\frac{\partial \varepsilon u_r}{\partial t}+\frac{1}{r}\frac{\partial(\varepsilon r u_r u_r)}{\partial r}+\frac{\partial(\varepsilon u_z u_r)}{\partial z}\right)=-\varepsilon\frac{\partial p}{\partial r}+\mu_f\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial(\varepsilon u_r)}{\partial r}\right)+\frac{\partial^2(\varepsilon u_r)}{\partial z^2}-\frac{\varepsilon u_r}{r^2}\right]+\bar{f}_{pr}\,, \tag{11}$$

$$\rho_f\left(\frac{\partial \varepsilon u_z}{\partial t}+\frac{1}{r}\frac{\partial(\varepsilon r u_z u_r)}{\partial r}+\frac{\partial(\varepsilon u_z u_z)}{\partial z}\right)=-\varepsilon\frac{\partial p}{\partial z}+\mu_f\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial(\varepsilon u_z)}{\partial r}\right)+\frac{\partial^2(\varepsilon u_z)}{\partial z^2}\right]+\bar{f}_{pz}+\varepsilon\rho_f\boldsymbol{g}\,, \tag{12}$$

where μ_f is the dynamic viscosity of the fluid, $\bar{f}_p=\dfrac{\int_0^{2\pi}\boldsymbol{f}_p\,d\theta}{2\pi}$ with f_{pr} and f_{pz} as its radial and axial components. From Eqs. (1)-(12), it can be seen that the two-way coupling in 3D-DEM/3D-CFD is still preserved in the simplified approach, and the only simplification is the averaging of fluid quantities over θ. From the formulation of $\bar{f}_p$, it can be known that the fidelity of the simplified approach is determined by the magnitude of the θ-component force and variation of r-component and z-component force along the tangential direction.

Finite volume method with staggered grid is used for discretization. For each time step of CFD, the porosity and pebble velocities from the DEM calculation are used to calculate the drag force using Eq. (7). Since the DEM time step is much smaller than the CFD time step, DEM solver and the CFD solver exchange data for every 100 DEM steps, with porosity and fluid properties invariant between data exchanging. The schematics of 3D-DEM/2D-CFD is shown in Fig. 1, where $\boldsymbol{F}_c=\boldsymbol{F}_n+\boldsymbol{F}_t$ is the pebble contact force.

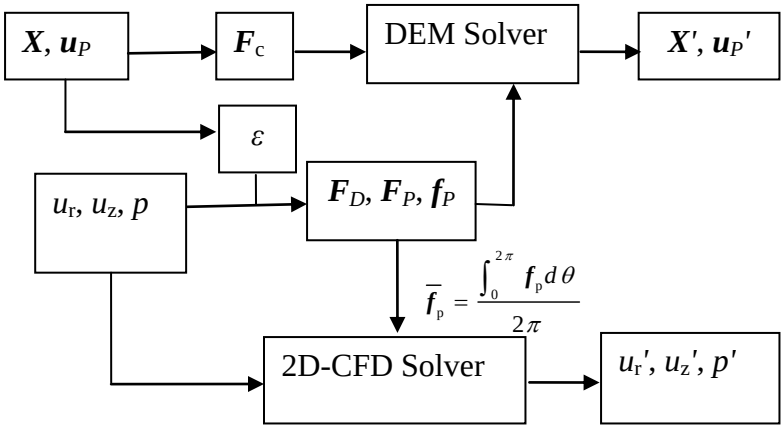
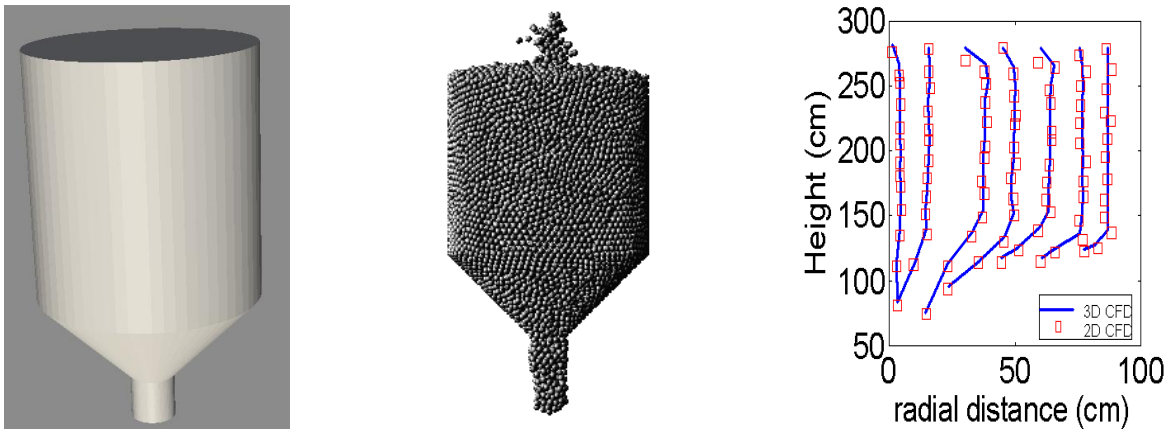


Figure 1. 3D-DEM/2D-CFD schematics

3. SIMULATION CONFIGURATION DESCRIPTION

The simulated problem originated from the HTR-10 project [13]. The reactor in the modeling has a radius of 90cm and the height of 252cm, with a 45 degree conic bottom and cylindrical chute. A total of 30K pebbles are randomly generated within the core using a collective dynamics-based initialization algorithm [14], with the packing fraction of around 61%. During the recirculation, pebbles are released from the bottom of the reactor through the chute, while new pebbles are inserted from the top of the reactor. Meanwhile, helium coolant is injected from the top of the reactor and emitted from the bottom of the reactor, with the boundary condition of constant velocity inlet and constant pressure outlet. The outside view of the reactor is shown as Figure 2(a) (generated by Paraview), and the physical parameters for the pebble and coolant are listed in Table I.



(a) simulation geometry **(b) simulation snapshot** **(c) typical pebble trajectories**

Figure 2. Reactor geometry and pebble initialization

Table I. Pebble and coolant physical properties

Pebble	Radius	Mass	Young's Modulus*	Friction Coefficient	Poisson Ratio
	3cm	210g	1e7 Pa	0.7	0.3
Helium Coolant*	Density	Dynamic viscosity	Specific heat	Inlet speed	Outlet Pressure
	6.132 g/L	3.86e-5 Pa.s	5.19e3 J/Kg.K	50 m/s	constant

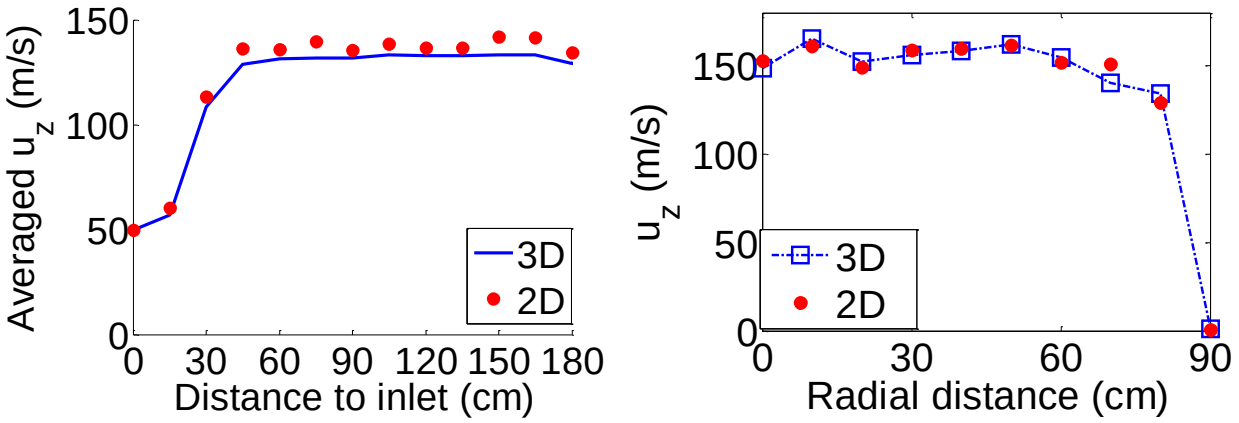
*: at 500 degrees Celsius, 100 bar.

The Young's Modulus adopted in the simulation is much smaller than the realistic 10^{10} Pa value for the pebble graphite surface material, which will allow for larger time step and speed up the simulation while basically keep the physical results unchanged [4]. And from Table I it can be calculated that the Mach number for the coolant flow is less than 0.2, therefore the incompressible assumption is valid.

4. RESULTS AND COMPARISONS

The circulating process of the pebbles is realized through the adoption of periodic boundary condition. For every pebble, once its position is below the surface of the outlet, it will recur from the top of the core. This periodic boundary condition is close to the realistic operation case and can well preserve the total quantity and motion balance of the pebble flow. For one fuel cycle, the full DEM-CFD simulation predicts 145s physical time for a fuel cycle, with the CPU time of around 10 days on Dell T7500 workstation. On the other hand, the simplified simulation gives the fuel cycle period of 139s, with the CPU time of only 3 days. Typical pebble trajectories starting from the same height but different radial position are shown in Figure 2(c) for both methods. From Figure 2(c) it can be observed that for pebble motion, the simplified approach well follow the result from the full 3D simulation.

After showing the pebble flow comparison, the fluid quantity contrast will be made as below. First the axial and radial profiles of vertical coolant velocity u_z (radially averaged) are given for both methods (Figure 3). It is clear to find from Figure 3(a) that the simplified method slightly overestimate u_z . Besides, a stable region for the u_z profile exists in the middle of the core. Figure 3(b) shows the radial profiles of u_z at the(h=100cm) from both method, showing no significant difference.



(a) axial profile of u_z **(b) radial profile of u_z**

Figure 3. Axial and radial profile of u_z

Another quantity of great interest is the overall pressure drop in the core along the axial direction, which is shown in Figure 4. The plot indicates that the 2D approach underestimates the pressure drop for 4% throughout the cylindrical core region.

The measured θ-component motions for both pebbles and coolant are typically two orders less than their z-component counterparts. Besides, the axial symmetry of the core geometry and the pebble packing distribution lead to small variation of r- and z-component pebble motion and coolant velocity along the tangential direction. As explained previously, these factors contribute to the fact the 2D result resembles the 3D simulation.

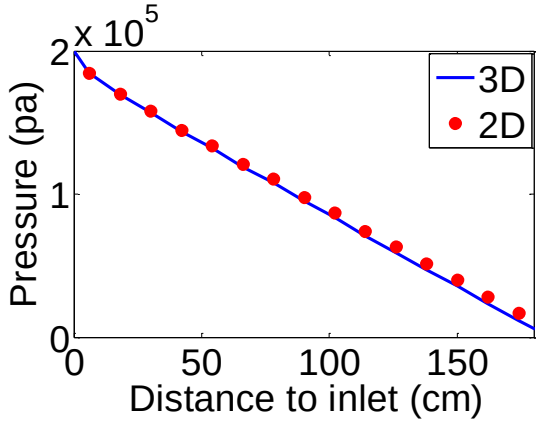


Figure 4. Pressure drop comparison

5. CONCLUSIONS

In this work, a simplified 3D-DEM/2D-CFD approach is proposed based on the axial symmetry of PBRs. Compared to the full 3D-DEM/3D-CFD simulation, the simplified approach can save more than 60% of CPU time for the HTR-10 geometry simulation. The axial symmetry of geometry and the pebble/coolant motion leads to insignificant accuracy loss during the averaging over the tangential direction. Deviations from the 3D simulation are inevitable, such as the overestimation of u_z and underestimation of pressure drop. However, these deviations are very slight and reproducible, which can be compensated in further simplified calculation.

By far the thermal and neutronic effect have not been included in the simulation, therefore it is important for this simplification on pebble-coolant modeling owing to its enhanced efficiency and relatively small loss of accuracy, which enable the potential to further incorporate other important physics in the PBR simulations.

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