SPH-DEM-Neutronics Coupling for Preliminary PBR Core Analysis

Joong Young Seo [a], Young Beom Jo [a], Eung Soo Kim [a*]
[a] Department of Nuclear Engineering, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul, South Korea
[*]Corresponding author: kes7741@snu.ac.kr

Keywords : Discrete Element Method, PBR, Heat transfer, Coupling, Smooth Particle Hydrodynamics

1. Introduction

Pebble Bed Reactor (PBR) is well known for its advantages in safety, refueling efficiency [1]. While such advantages come from the packed structure, the random distribution of pebbles makes it challenging to model and simulate the core. While the change in the packed state of pebble beds could lead to unexpected events such as avalanches and jamming [2], it would also affect the neutron moderations, affecting the multiplication factor [3].

Therefore, a Multiphysics analysis on the transient behavior of pebble beds should be conducted at a particle scale due to the high sensitivity of PBR behavior on core structure. In this respect, discrete element method (DEM) based on contact mechanics can be a powerful option for tracking pebbles, providing accurate information on pebble packing and velocity.

In this study, a particle-based analysis for such granular systems has been developed by coupling the SPH model and DEM model with an internal conduction model to consider heat transfer within the pebble with validations. Then, a simplified analysis of a PBR core has also been conducted by coupling with a neutronics code. GPU parallelization were applied to the codes for acceleration, using NVIDIA's CUDA architecture [4][5].

2. Numerical Methods

The numerical models used in this study to model the multiphase interactions will be introduced in this section. Smooth Particle Hydrodynamics (SPH) will be used for the CFD method, while Discrete Element Method (DEM) will be used to simulate granular solid behavior.

2.1 Smooth Particle Hydrodynamics (SPH)

Smooth Particle Hydrodynamics (SPH) represent the fluid system as a set of particles. Physical quantities are assigned to each particle, calculated as the weighted average of neighboring particles within the support domain. A kernel function that resembles the delta function is used for averaging. Equation (1) is a SPH discretization of a function f at particle i. V is the particle volume, and W_{ij} is the kernel function value for neighboring particle j.

$$f(r_i) = \sum_j f(r_j) W_{ij} V_j \tag{1}$$

The main principles of such interpolations are described in Fig. 1.

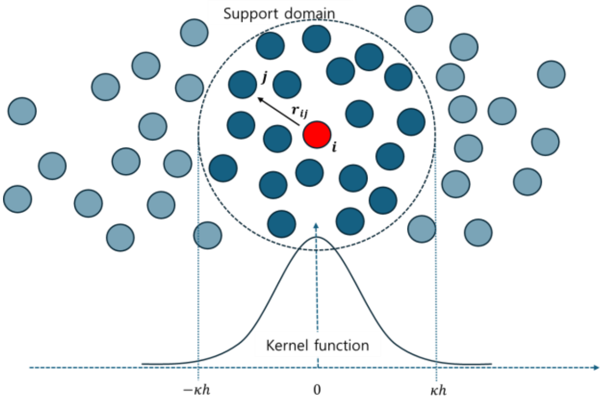

Fig. 1. SPH interpolation method

2.2 Discrete Element Method

Discrete Element Method (DEM) is a numerical approach to analyze the behavior of solid particles. The total interaction acting on each particle is calculated individually in a discrete manner, allowing the accurate prediction of granular system behavior.

2.2.1 Mechanical DEM

The linear/angular velocities of each particle are updated using Newton's Second Law of motion. To calculate the forces due to collisions, a spring-dashpot model based on the soft sphere approach were implemented. Slight overlaps between particles are allowed where the colliding part is treated as a system of a spring and a damper, shown in Fig. 2.

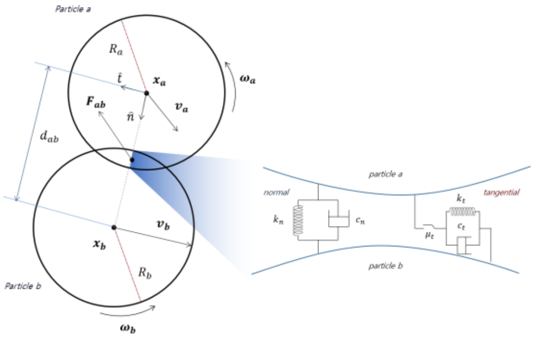

Fig. 2. Spring-dashpot model

From the spring-dashpot model, normal and tangential forces can be expressed using overlap length δ.

$$\overrightarrow{\boldsymbol{f_c}} = (k_n\delta_n - c_n|\overrightarrow{\boldsymbol{v_{cn}}}|\boldsymbol{\hat{n}} + f_s\boldsymbol{\hat{s}} \tag{2}$$

$$f_s = min(k_s\delta_s - c_s|\overrightarrow{\boldsymbol{v_{cs}}}|, f_{\boldsymbol{friction}}) \tag{3}$$

In this study, the Hertz Mindlin contact model was applied to determine the elastic, damping terms. Effective values of Young's modulus, Shear modulus, radius and mass$(\mathrm{E}, \mathrm{G}, \mathrm{R}, \mathrm{m})$ were used to describe the collision.

Table 1. DEM collision model

Normal Force Term ($\boldsymbol{f^n}$)
$\boldsymbol{k_n} = \frac{4}{3}E_{ij}{}^*\sqrt{R_{ij}{}^*}\ \delta_n{}^{3/2}$
$\boldsymbol{c_n} = \sqrt{\frac{\mathbf{10}}{\mathbf{3}}}\frac{\mathbf{ln}(\boldsymbol{e})}{\sqrt{\boldsymbol{ln}(\boldsymbol{e})^{\mathbf{2}} + \boldsymbol{\pi}^{\mathbf{2}}}}\sqrt{M_{ij}{}^*2E_{ij}{}^*\sqrt{R_{ij}{}^*\delta_n}}$
Tangential Force Term ($\boldsymbol{f^t}$)
$\boldsymbol{k_s} = \mathbf{8}\boldsymbol{G_{ij}}{}^*\sqrt{\boldsymbol{R_{ij}}{}^*\boldsymbol{\delta_n}}$
$\boldsymbol{c_s} = \sqrt{\frac{\mathbf{10}}{\mathbf{3}}}\frac{\boldsymbol{ln}(\boldsymbol{e})}{\sqrt{\boldsymbol{ln}(\boldsymbol{e})^{\mathbf{2}} + \boldsymbol{\pi}^{\mathbf{2}}}}\sqrt{M_{ij}{}^*k_s}$

2.2.2 Thermal DEM

Similarly, the temperatures of each particle are updated by calculating transferred heat. Conductive heat transferred between stationary particles i, and j can be expressed as equation (4).

$$Q_{ij} = 2k\left(\frac{3F_nR_{ij}^*}{4E_{ij}^*}\right)^{1/3}(T_i - T_j) \tag{4}$$

Therefore, a one dimensional internal heat conduction was also considered in this study, shown in Fig. 3.

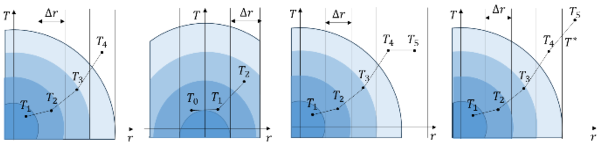

Fig 3. Internal conduction model

Fourier heat equation was discretized using Finite Differential Method(FDM) shown in equation (5).

$$\begin{aligned}\rho c_p\frac{\partial T_i}{\partial t} = \frac{\partial k}{\partial T}\left(\frac{T_{i+1} - T_{i-1}}{2\Delta r}\right)^2 \\ + \frac{2}{r_i}k\left(\frac{T_{i+1} - T_{i-1}}{2\Delta r}\right) \\ + k\frac{T_{i+1} - 2T_i + T_{i-1}}{(\Delta r)^2} \\ + O((\Delta r)^2)\end{aligned} \tag{5}$$

Thermal expansion was also modeled using FDM assuming isotropic radial expansion for simplicity. 1D radial expansion rate is obtained from the temperature change rate, based on the definition of 1D heat expansion coefficient. α_L.

$$\frac{dR}{dt} = R\alpha_L\frac{dT}{dt} \tag{6}$$

For radiative heat transfer, simplifications were made to the previous short-range radiation model [6]. The spheres are assumed to be grey emitting, were emissivity ε_{pi} is used to calculate the transferred heat, shown in equation (7). Y_{ij} is the view factor of the system.

$$Q_{ij} = \frac{\sigma(T_i^4 - T_j^4)}{\frac{1 - \varepsilon_{pi}}{\varepsilon_{pi}A_i} + \frac{1}{A_iY_{ij}} + \frac{1 - \varepsilon_{pj}}{\varepsilon_{pj}A_j}} \tag{7}$$

Here, only particles within the effective radiation range are assumed to transfer radiative heat. The value for the effective radiative range will be discussed later.

3. SPH-DEM coupling for multiphase systems

The multiphase system of a PBR core was modeled using SPH method for the fluid and DEM calculations for the solid pebble fuels. An unresolved coupling between two methods were adopted. In this approach, overlaps between SPH and DEM particles are allowed, where heat and momentum transfer between two phases occurs. The fundamental concept of such approach is described in Fig. 4.

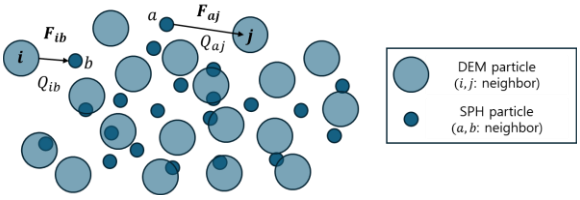

Fig. 4. Unresolved SPH DEM coupling

The interaction to solid DEM particles is estimated from adjacent SPH particles. Then the forces and heat acting on SPH particles are calculated based on Newton's third law. Then the resulting forces acting on DEM particles and the SPH discretized form of fluid equations at multiphase situations are shown in Table 2,3.

Table 2. DEM interactions

Momentum Equations
$\left(\frac{d\boldsymbol{u}}{dt}\right)_i = \rho_i\boldsymbol{g} + \sum_b \boldsymbol{F_{ib}}$
Energy Equations
$\bar{\rho}_ic_{p,i}\frac{dT_i}{dt} = \sum_b Q_{ib}W_{ib}$

Table 3. SPH interactions

Momentum Equations
$(\frac{d\boldsymbol{u}}{dt})_a = -\sum_b \overline{m}_b \left(\frac{p_a}{\overline{\rho}_a^2} + \frac{p_b}{\overline{\rho}_b^2}\right) \nabla_a W_{ab} + \overline{\rho_a} g + \boldsymbol{S_a}$
Energy Equations
$< c_p \frac{dT}{dt} >_a = \sum_b \frac{\overline{m_b}}{\rho_a \rho_b} \left(\frac{4\overline{k_a k_b}}{\overline{k_a} + \overline{k_b}}\right) (T_a - T_b) \nabla_a W_{ab} + \frac{1}{\overline{\rho_a}} \sum_j \left(\frac{W_{aj}}{\sum_{b'} \frac{m_{b'}}{\rho_{b'}} W_{jb'}}\right) Q_j$

The force term $\boldsymbol{F}$ and $\boldsymbol{S}$ represents the coupling force acting on DEM and SPH particles.

The over lined parameters are superficial values, where the local porosity is multiplied. The local porosity of SPH particle a can be expressed as below.

$$\varepsilon_a = 1 - \sum_j W_{aj} V_{\mathrm{j}} / \sum_b W_{ab} V_b \tag{8}$$

The momentum transfer is calculated from the local pressure gradient θ and buoyancy force, and the transferred heat can be obtained using the convective heat equation. The results are shown in equation (9), and (10). $f(\varepsilon)$ is the porosity function of the system.

$$\boldsymbol{F_{ib}} = V_i \sum_b \left(\frac{m}{\rho}\right)_b \theta_b W_{ib} + \frac{1}{8} C_d \rho_f A |\boldsymbol{u_{bi}}| \boldsymbol{u_{bi}} f(\varepsilon) \tag{9}$$

$$Q_{ib} = (2.0 + 0.6 Re_b^{\frac{1}{2}} Pr^{\frac{1}{3}}) \frac{6k}{d^2} (T_b - T_i) \tag{10}$$

4. Validations of numerical simulations

Validations for the SPH DEM coupled simulations has been performed. Details will be covered in this section.

4.1 DEM heat transfer model

Comparisons with the experimental data of measuring the effective thermal conductivity at vacuum was conducted for the validation of DEM heat transfer model.

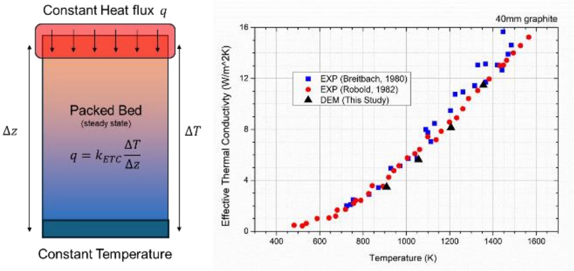

Fig. 5. DEM heat transfer validation

The effective radiation range of $3.5r_p$ showed high accuracy for graphite and ZrO_2 packed beds. Therefore, it can be concluded that the assumption of effective radiation range is valid.

4.2 SPH-DEM coupled model

The validation of SPH-DEM coupling was conducted in both mechanical and thermal perspectives. For the modeling of hydrodynamic interactions, the pressure drop of flow through the packed bed was compared with predictions from Ergun's equation.

As shown in Fig. 6, the numerical results showed good agreements with the analytic/experimental data.

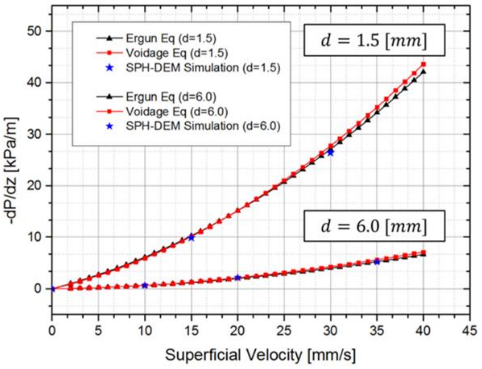

Fig. 6. Validation of SPH-DEM interactions

5. Preliminary analysis of a PBR core

An initial stage coupling of DEM and neutronics code was applied to simulate the pebble-scale behavior of PBR operation. The HTR-10 core was modeled and analyzed in this study. The packed state of pebble data is obtained by DEM model, which is exported as an input to PRAGMA, a reactor physics code [7].

Based on the given data, the heat generation of individual pebbles can be exported, given to the DEM code for mechanical/thermal calculations. The concept and procedure are shown in Fig. 7.

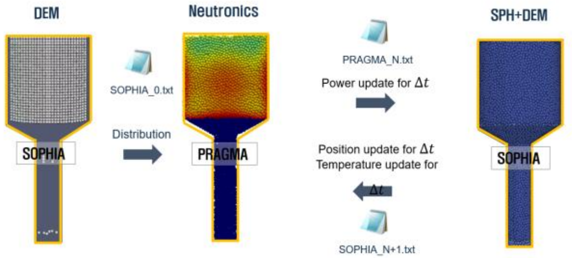

Fig. 7. DEM neutronics coupling for HTR-10 core

A reactor operating in vacuum was considered in this section. Such events could happen in case of a Depressurized Loss of Forced Coolant (DLOFC) accident, where rapid loss of coolant gas occurs due to a rupture. In such situations, the effects of coolant are removed, leading to extremely high temperature and the risk of fuel failure in the reactor. For simplicity, an extreme coolant loss was assumed along with the initiating operation of the reactor.

Transient analysis was conducted for different power levels (100%, 10%, 1%, 0.1% of PRAGMA data). The initial temperature of pebbles was set to 298K, while the exterior part of the core was kept isothermal for the boundary condition.

The resulting temperature distribution due to the power input was observed at the steady state, with the maximum temperature exceeding 3500K at 100% power simulations. At high power conditions, local porosity was found to have notable differences for different power and positions. The results are shown in Fig. 8.

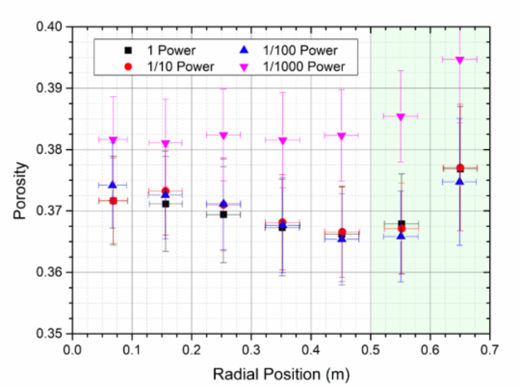

Fig. 8. Transient effects on HTR-10 core

Such results imply that heat expansion in high temperature situations has a significant influence on the packed state of pebbles. Since there is a possibility of heat transfer change due to such geometrical shifts, a thorough analysis regarding the anisotropic expansion of pebbles may be required in further works for more accurate predictions.

6. Summary

In this study, a DEM model that covers both external and internal heat transfer is introduced with validations. Then, coupling DEM code with the SPH method is conducted to simulate mechanical/thermal interaction at multiphase systems, along with validations. A neutronics code is coupled with the modified DEM code to simulate simplified PBR structure at the loss of coolant, where significant changes in local porosities due to temperature and power distributions are observed. In conclusion, the feasibility of coupling DEM with other codes were achieved, suggesting future works of modeling a more detailed PBR system for a more realistic analysis.

,

Acknowledgement

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT). (No. 2021M2D2A1A03046881)

References

[1] Kadak, A. C. (2005). A future for nuclear energy: pebble bed reactors. *International journal of critical infrastructures*, *1*(4), 330-345.

[2] Park, S. S., & Kim, E. S. (2020). Jamming probability of granular flow in 3D hopper with shallow columns: DEM simulations. *Granular Matter*, *22*(4), 77.

[3] Niu, B., Ahmed, M., Wen, T., Xu, G., & Liu, X. (2023). Particle-resolved CFD modeling of the flow and heat transfer characteristics of the fluid in a fixed bed. *Powder Technology*, *421*, 118445.

[4] Jo, Y. B., Park, S. H., Choi, H. Y., Jung, H. W., Kim, Y. J., & Kim, E. S. (2019). SOPHIA: Development of Lagrangian-based CFD code for nuclear thermal-hydraulics and safety applications. Annals of Nuclear Energy, 124, 132-149.

[5] Jo, Y. B., Park, S. H., Yoo, H. S., & Kim, E. S. (2022). GPU-based SPH-DEM Method to Examine the Three-Phase Hydrodynamic Interactions between Multiphase Flow and Solid Particles. International Journal of Multiphase Flow, 153, 104125.

[6] Cheng, G. J., & Yu, A. B. (2013). Particle scale evaluation of the effective thermal conductivity from the structure of a packed bed: radiation heat transfer. *Industrial & engineering chemistry research*, *52*(34), 12202-12211.

[7] Choi, N., Kim, K. M., & Joo, H. G. (2021). Optimization of neutron tracking algorithms for GPU-based continuous energy Monte Carlo calculation. *Annals of Nuclear Energy*, *162*, 108508.