PRESENTATION TITLE
Review of the Prospectus of the Dissertation

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STRUCTURE

1. Introduction

2. Literature Review

3. Development of Modeling Tools for Pebble Bed Morphological Evolution Studies

4. Studies of Pebble Bed Thermophysics, Mechanics, & Morphological Changes

INTRO.

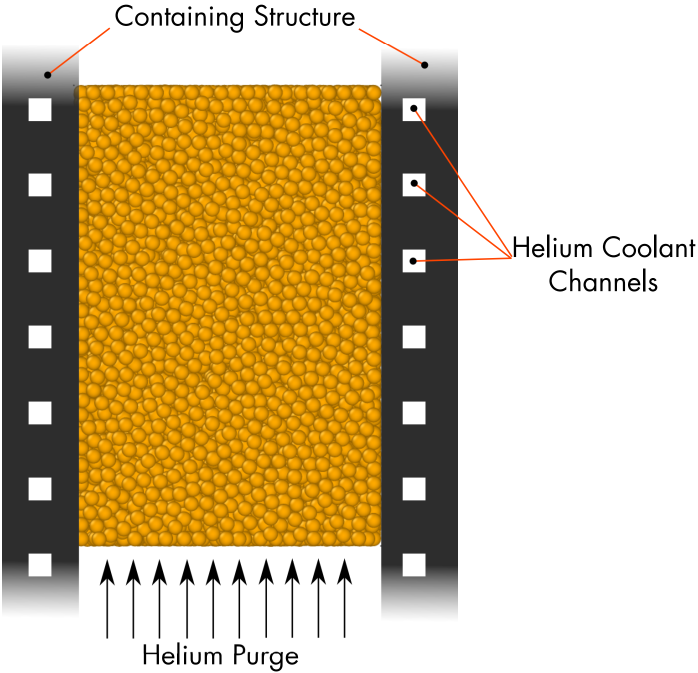
BACKGROUND AND MOTIVATION

Many solid breeder designs are now employing a **breeder unit** configuration

- Packed sub-modules of ceramic pebble beds
- Units individually tested experimentally and qualified during design phase

Must understand how packing states may evolve from time-dependent phenomena (e.g. pebble damage from crushing, sintering, creep, etc.)

- Decrease in effective thermal conductivity raises bed temperatures
- Pebble isolation creating hot spots and sintering – potentially decreasing tritium release rates
- Gap formation decreases interfacial heat conductance and leads to neutron streaming, etc.


Containing Structure
Helium Coolant Channels
Helium Purge

MODELING TECHNIQUES

Discrete element method

Particle-scale information of forces and temperatures for modeling and predicting pebble damage

Coupled computational fluid dynamics and discrete element method

Volume-averaging fluid flow for efficient simulations of large volumes with transient, coupled modeling to pebble-scale DEM computations

Lattice-Boltzmann method

Interrogate the entire, tortuous flow path with efficient modeling of fluid flow through geometrically complex packing structures

LIT. REVIEW

MODEL DEV.

PARTICLE DYNAMICS

Track particle trajectories,

$$m_i \frac{\mathrm{d}^2 \mathbf{r}_i}{\mathrm{d}t^2} = m_i \mathbf{g} + \sum_{j=1}^{Z} \mathbf{f}_{n,ij} \qquad (1)$$

$$\mathbf{f}_{n,ij} = k_{n,ij} \delta_{n,ij} \mathbf{n}_{ij} - \gamma_{n,ij} \mathbf{u}_{n,ij} \qquad (2a)$$

$$k_{n,ij} = \frac{4}{3} E^*_{ij} \sqrt{R^*_{ij} \delta_{n,ij}} \qquad (2b)$$

$$\frac{1}{R^*_{ij}} = \frac{1}{R_i} + \frac{1}{R_j} \qquad (3a)$$

$$\frac{1}{E^*_{ij}} = \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j} \qquad (3b)$$

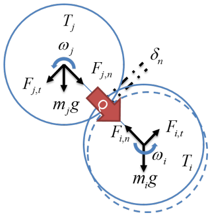


Figure: Allowing fictive overlap, δ, between centroids to determine repulsive force between pebbles.

Equations of motion are integrated with the Velocity-Verlet algorithm – global error of approximately $O(\Delta t^2)$

PARTICLE HEAT TRANSFER

$$m_i C_i \frac{\mathrm{d}^2 T_i}{\mathrm{d}t^2} = Q_{s,i} + \sum_{j=1}^{Z} H_c(T_i - T_j) \tag{4}$$

$$H_c = 2k^* \left[\frac{3F_{n,ij}R^*}{4E^*}\right]^{1/3} \tag{5}$$

$$d_{p,i} = d_{p_0,i}\left[1 + \beta_i\left(T_i - T_{\text{ref}}\right)\right] \tag{6}$$

PARTICLE IN FLUID FIELD

Add a drag on particle due to passing fluid and energy exchange at the interface. Eqs. 1 and 4 become,

$$m_i \frac{\mathrm{d}^2 \mathbf{r}_i}{\mathrm{d}t^2} = m_i \mathbf{g} + \sum_{j=1}^{Z} \mathbf{f}_{n,ij} + \beta_i V_i \Delta \mathbf{u}_{if} \tag{7a}$$

$$m_i C_i \frac{\mathrm{d}^2 T_i}{\mathrm{d}t^2} = Q_{s,i} + \sum_{j=1}^{Z} Q_{ij} + \beta_{E,i} A_i \Delta T_{if} \tag{7b}$$

the inter-phase exchange coefficients are defined as

$$\beta_i = \frac{18\mu_f}{d_{p,i}^2}(1 - \phi_k)\phi_k F \tag{8a}$$

$$\beta_{E,i} = \frac{\mathrm{Nu} k_f}{d_{p,i}} \tag{8b}$$

NON-DIMENSIONAL DRAG CORRELATIONS

Koch, Hill, & Ladd provide non-dimensional drag as

$$F = F_0(\phi) + F_3(\phi)\mathrm{Re} \tag{9}$$

where

$$F_0 = \begin{cases} \frac{1+3(\phi/2)^{1/2}+(135/64)\phi\ln\phi+16.14\phi}{1+0.681\phi-8.48\phi^2+8.16\phi^3} & \text{if } \phi < 0.4 \\ 10.0\,\frac{\phi}{(1-\phi)^3} & \text{if } \phi > 0.4 \end{cases} \tag{10a}$$

$$F_3 = 0.0673 + 0.212\phi + 0.0232\frac{1}{(1-\phi)^5} \tag{10b}$$

Li & Mason provide Nusselt number as

$$\mathrm{Nu} = \begin{cases} 2 + 0.6\epsilon^n \mathrm{Re}_p^{1/2}\mathrm{Pr}^{1/3} & \mathrm{Re}_p < 200 \\ 2 + 0.5\epsilon^n \mathrm{Re}_p^{1/2}\mathrm{Pr}^{1/3} + 0.02\epsilon^n \mathrm{Re}_p^{0.8}\mathrm{Pr}^{1/3} & 200 < \mathrm{Re}_p < 1500 \\ 2 + 0.000045\epsilon^n \mathrm{Re}_p^{1/2} & \mathrm{Re}_p > 1500 \end{cases} \tag{11}$$

where they found from experiments that $n = 3.5$ was appropriate for 3 mm polymer pellets in dilute flows

FLUID CONSERVATION EQUATIONS

Volume-averaged Navier-Stokes and Energy equations with closure terms from DEM data,

$$\frac{\partial \epsilon_k \rho_f}{\partial t} + \nabla \cdot (\epsilon_k \mathbf{u}_f \rho_f) = 0 \tag{12a}$$

$$\frac{\partial \epsilon_k \mathbf{u}_f}{\partial t} + \nabla \cdot (\epsilon_k \mathbf{u}_f \mathbf{u}_f) = -\frac{\epsilon_k}{\rho_f} \nabla P_f + \nabla \cdot (\nu_f \epsilon_k \nabla \mathbf{u}_f) - \frac{\mathbf{S}_k}{\rho_f} \tag{12b}$$

$$\frac{\partial \epsilon_k T_f}{\partial t} + \nabla \cdot (\epsilon_k \mathbf{u}_f T_f) = \nabla (\epsilon_k \nabla T_f) - \frac{E_k}{\rho_f C_f} \tag{12c}$$

Coupling the fluid phase to the particles happens with the sink terms in momentum and energy of $\mathbf{S}_k$ and E_k

$$\phi_k = 1 - \epsilon_k = \frac{1}{V_k} \sum_{\forall i \in k} V_{p,i} \tag{13a}$$

$$\mathbf{S}_k = \frac{1}{V_k} \sum_{\forall i \in k} \beta_i V_i \Delta \mathbf{u}_{if} \tag{13b}$$

$$E_k = \frac{1}{V_k} \sum_{\forall i \in k} \beta_{E,i} A_i \Delta T_{if} \tag{13c}$$

LAGRANGIAN-EULERIAN MAPPING

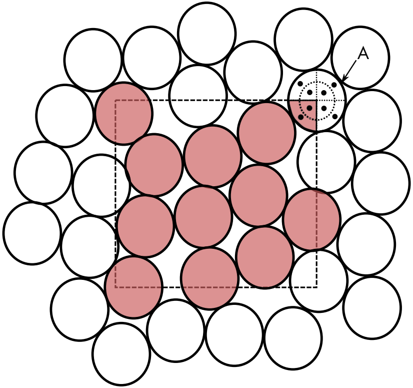


Figure: The dashed line represents a computational cell in which exist many particles. The particles with centroids inside the cell are shaded red.

$$\epsilon_{\text{cell}} = 1 - \frac{1}{V_{\text{cell}}} \sum_{i=A}^{i=L} w_i V_{p,i} \tag{14}$$

LATTICE-BOLTZMANN INTRODUCTION

Discretize the continuous

BHATNAGAR-GROSS-KROOK LATTICE-BOLTZMANN FORMULATION

$$\underbrace{f_i(\mathbf{x}+\mathbf{c}_i, t+1) = f_i(\mathbf{x}, t)}_{\text{streaming}} + \underbrace{\Omega_i(\mathbf{x}, t)}_{\text{collision}} \tag{15}$$

The collision operator is calculated based only on each nodes local information. Using the single-relaxation time BGK approximation the collision is calculated as

$$\Omega_i = -\frac{1}{\tau}\left[f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t)\right] \tag{16}$$

Relaxation towards the equilibrium distribution function

$$f_i^{\text{eq}} = \rho(\mathbf{x}, t) w_i \left[1 + \frac{\mathbf{u}\cdot\mathbf{c}_i}{c_s^2} + \frac{(\mathbf{u}\cdot\mathbf{c}_i)^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2}\right] \tag{17}$$

Bounce-back boundary condition

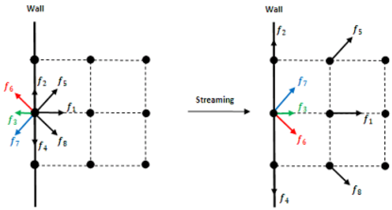


Figure: Sketch of the D2Q9 nodes showing at the boundary the distribution functions that would come from neighbors outside the boundary (at the wall) are unknown (drawing from correspondence with Dr. Bao, billbao@cims.nyu.edu).

$$\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t) \tag{18a}$$

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x}, t)} \sum_i \mathbf{c}_i f_i(\mathbf{x}, t) \tag{18b}$$

The fluid pressure is related to the density for an ideal gas, so we can find the physical pressure in terms of the lattice density,

$$p = p_0 \frac{\rho(\mathbf{x}, t)}{\rho_0} \tag{19}$$

STUDIES