A fixed coarse-grid thermal-fluid scheme and a heat conduction scheme in the distinct element method

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Abstract

A particle-thermal-fluid coupling scheme with a mixed Lagrangian-Eulerian approach is described by extending the author’s previous research (Shimizu, 2004). The scheme solves the continuity, Navier-Stokes (N-S) and thermal energy equations numerically in Eulerian Cartesian coordinates by considering the existence of particles within the cell. On the other hand, in the Distinct Element Method (DEM), driving forces and thermal energy applies to the particles.

Keywords: particle-thermal-fluid coupling, mixed Lagrangian-Eulerian approach, distinct element method.

1 Introduction

Numerical analysis of particle-fluid coupling using a mixed Lagrangian-Eulerian approach is becoming popular, especially in the chemical and mechanical engineering fields [5,6,8]. Also, this approach has many potential applications in the geo-engineering field especially when there is a wide range of fluid velocity and high porosity [7]. In this scheme, the fluid phase is described by using the continuity and momentum (Navier–Stokes) equations to calculate pressure and velocity of fluid, while the movement of the solid phase (particles) is traced by the DEM as a Lagrangian method. Momentum exchange between particles and fluid is considered in the momentum equation for the fluid phase and in the force-displacement law for the solid phase. Here, we extend the mixed Lagrangian-Eulerian approach to include the thermal energy equation to solve for temperature in both fluid and particles. A correlation of forced convection heat transfer by considering particle existence is used for interaction term.
between particles and fluid in thermal energy equation for fluid-phase. Also, the interaction term is added as a source term in the heat transfer equation for solid-phase (particles). In this paper, the complete scheme, as implemented on PFC$^{2D}$ and PFC$^{3D}$ [3,4], is described, with especial emphasis on the interaction term. Two-dimensional simulations with forced convection heat transfer are conducted.

2 Interaction between particles and fluid by forced convection heat transfer

Figure 1 shows a fixed control volume $\Delta x \Delta y \Delta z$ in the model, in which $N_p$ spherical particles exist within a flowing fluid, the temperature is $T_f$. Each particle has a temperature $T_{p_n} (n: 1, N_p)$, and the average temperature is $T_b (\equiv \overline{T_{p_n}})$. There is no temperature variation within each particle.

Consider thermal energy exchange between the particle assembly (bulk material) and fluid, by forced convective heat transfer. The thermal energy flux per unit volume caused by temperature difference between particle assembly and fluid $Q_{\text{int}} \ [\text{W/m}^3]$ is given by eq.(1). Here, the heat-transfer coefficient and average particle temperature are defined in each control volume.

$$Q_{\text{int}} = h_b \left( T_b - T_f \right) \pi \sum_{n=1}^{N_p} d_{p_n}^2 \Delta x \Delta y \Delta z = \frac{6h_b(1 - \varepsilon)}{d_p^3} \left( T_b - T_f \right)$$ (1)

Figure 1: Fluid flow with thermal energy through particle assembly.
where
\[ d_{p_a} : \text{particle diameter (n=1,Np)} \quad \text{[m]} \]
\[ h_b : \text{heat-transfer coefficient of particle assembly} \quad \text{[W/m}^2\text{.K]} \]
\[ T_b : \text{temperature of particle assembly} \quad \text{[K]} \]
\[ T_f : \text{temperature of fluid} \quad \text{[K]} \]
\[ \varepsilon : \text{porosity} \quad [-] \]

The heat-transfer coefficient of particle assembly \( h_b \) is usually provided by empirical equations, which depend on material properties, flow condition and particle arrangement (porosity). One such relation for heat transfer by forced convection is given by eq. (2) [9]. This empirical equation is derived by using air, and is applicable for porosity, \( \varepsilon \), below 0.8.

\[
h_b = \frac{k_f}{d_p} \left( 1 - \varepsilon \right) \left( \frac{0.5 \left( \frac{\text{Re}}{1 - \varepsilon} \right)^{\frac{1}{2}} + 0.2 \left( \frac{\text{Re}}{1 - \varepsilon} \right)^{\frac{2}{3}} \right) \frac{\text{Pr}^{\frac{1}{3}}}{\varepsilon \leq 0.8} \tag{2} \]

where \( \text{Re} \) is the particle Reynolds number and \( \text{Pr} \) is the Prandtl number defined by eq. (3) and (4).

\[
\text{Re} = \frac{\bar{\mathbf{u}}_\text{rel}}{\mu_f} \left[ \frac{d_p \varepsilon \rho_f}{\bar{\mathbf{v}} - \mathbf{u}} \right] = \frac{\bar{\mathbf{v}} - \mathbf{u}}{\mu_f} \left[ \frac{d_p \varepsilon \rho_f}{\mu_f} \right] \tag{3} \]

\[
\text{Pr} = \frac{c_f \mu_f}{k_f} \tag{4} \]

\( c_f : \text{specific heat} \quad \text{[J/kg.K]} \]
\( d_{p_a} : \text{average particle diameter} \quad \text{[m]} \]
\( k_f : \text{thermal conductivity} \quad \text{[W/m}^2\text{.K]} \]
\( \mathbf{u} : \text{fluid velocity vector} \quad \text{[m/s]} \]
\( \bar{\mathbf{v}} : \text{average particle velocity vector} \quad \text{[m/s]} \]
\( \mu_f : \text{viscosity} \quad \text{[Pa.s]} \]
\( \rho_f : \text{density of fluid} \quad \text{[kg/m}^3\text{]} \]
The thermal energy flux applied to the particle assembly within the control volume, $Q_{apb}$, is given as a form of preserving the thermal energy exchange between particle assembly and fluid. The $Q_{apb}$ is also sum of the rate of thermal energy applied to each particle. Hence,

$$Q_{apb} = \sum_{n=1}^{N_p} Q_{apb,n} = -Q_{int} \Delta x \Delta y \Delta z = h_b \left( T_f - T_b \right) \pi \sum_{n=1}^{N_p} d_{pn}^2$$

(5)

Hence, the rate of thermal energy applied to each particle due to convective heat transfer $Q_{apb,n}$ is given by eq. (6).

$$Q_{apb,n} = h_b \left( T_f - T_b \right) \pi d_{pn}^2$$

(6)

3 Formulation and scheme

The thermal scheme for the fluid-phase is invoked between application of the Law of Motion and the Force-Displacement Law in the mechanical (DEM) calculation, with the interaction forces on particles being added as external body forces in the mechanical calculation. Also, the thermal scheme for the particle-phase is invoked after the thermal-fluid scheme, so that temperatures of all particles are updated.

3.1 Fluid-phase, thermal-fluid scheme

The continuity, Navier Stokes equation and thermal energy equation for fluid-phase in the fluid-solid two-phase flow model (using incompressible fluid with constant density) are given by eqs. (7) and (8) [7]. Also the thermal energy equation is given by eq. (9).

$$\frac{\partial \varepsilon}{\partial t} = -\left( \nabla \cdot \varepsilon \mathbf{u} \right)$$

(7)

$$\frac{\partial (\varepsilon \mathbf{u})}{\partial t} = -\left( \nabla \cdot \varepsilon \mathbf{uu} \right) - \frac{\varepsilon}{\rho_f} \nabla p + \frac{f_{int}}{\rho_f}$$

(8)

$$\frac{\partial (\varepsilon T_f)}{\partial t} = -\left( \nabla \cdot \varepsilon T_f \mathbf{u} \right) + \frac{k_f}{\rho_f c_f} \nabla^2 \left( \varepsilon T_f \right) + \frac{Q_{int}}{\rho_f c_f}$$

(9)
where

\[ f_{\text{int}} : \quad \text{interaction force per unit volume} \quad \text{[N/m}^3\text{]} \]

The natural convection term is not included in eq. (8), since forced convection is dominant in the simulations considered here. Also, the viscous term is not included. The interaction force per unit volume is calculated by using a fluid-particle friction coefficient. Also, the driving force applied to a particle is calculated by using the interaction force and pressure gradient [7].

### 3.2 Particle-phase, thermal scheme

The conduction heat transfer is applied through particle-particle contacts, and is described in the code user’s manuals [3,4]. Each particle exchanges thermal energy between neighbor particles through a thermal pipe created between two contacted particles with a thermal resistance (Fig. 2). Also, the rate of thermal energy due to convection heat transfer \( Q_{ap} \) (eq. (6)) is added to the particle as one of the source term.

![Figure 2: Network of particle assembly.](image)

4 Simulations

Two simulations are performed. The first verifies the interaction term for convective heat transfer. A simple two-dimensional model with regularly arranged particle is created in order to observe the transient particle temperatures and the result is compared with the analytical solution. The other simulation is an application example; a gas-fluidized bed simulation. Gas is introduced into a particle assembly to study the migration and temperature transient of each particle.
4.1 Two-dimensional fixed particles case

Figure 3 shows the particle arrangement and the fluid cells placed in the model. The model dimensions are 0.096 m width and 0.12 m height. 80 particles with 10mm diameter are placed as regular arrangement. There are no contacts between particles, to prevent conduction heat transfer through contact points. 80 fluid cells (8 x 10) are created as occupying one particle in each cell. Extra cells are created at the outside in order to take account of boundary conditions. The dimension of each cell is 12 mm in the x and y direction, and the porosity of each fluid cell is 0.64. Slip-wall boundary (fluid velocity parallel to the boundary surface is non-zero at the boundary) is specified at the side boundary, and a zero pressure boundary is specified at the top boundary, from which fluid discharges. A fluid velocity is specified at the bottom boundary to create a uniform velocity profile. Thermally adiabatic boundary condition: there is no thermal energy transfer across boundaries, is specified at the side boundary. At the bottom boundary, the fluid temperature is set to 100 K. The time step for both of the DEM and the thermal-fluid calculation is taken as $5.0 \times 10^{-5}$ s.

Table 1 shows the material properties. The material properties for particle are not related to a real material, because the objective of this simulation is to verify heat transfer between particles and fluid in the scheme.

![Figure 3: Model: particle assembly and fluid cell.](image_url)
The simulation procedure is as follows. First, particles with 0 K temperature are created in a regular arrangement, with translational and rotational movements being prevented. Second, while heat transfer between particle and fluid is turned off, air is injected at 1.0 m/s of apparent velocity from the bottom boundary during 3000 cycles to make a constant flow profile and 100 K of each fluid cell temperature. After that, by fixing the air temperature for all fluid cells, the heat transfer between particles and fluid is turned on in order to study the evolution of temperature. A measurement area is set, to trace fluid and particle temperatures.

Figure 4 shows the time history of particle and fluid temperature. Solid line shows the analytical value calculated by an equation in the figure, which is derived from the particle thermal equation without conduction heat transfer term. The numerical result is in good agreement with the analytical solution.

![Figure 4: Comparison between simulation result and analytical value: transient of particle temperature, 0–40 s.](image)
4.2 Two-dimensional fluidized bed simulation

Figure 5 shows the particle assembly and the fluid cells placed in the model. The model consists of particles and surrounding walls. The model dimensions are 0.15 m width and 0.6 m height, surrounded by bottom and side walls. 2400 particles with 4 mm diameter are created within the walls. The assembly height is around 0.22 m. 450 fluid cells (15 x 30 (width x height)) are created, with a cell size of 10 and 20 mm respectively. Slip-wall boundary is specified at the side and bottom boundary, and a zero pressure boundary is specified at the top of the boundary. A fluid velocity is specified at the center of the bottom boundary, from which fluid with temperature 1000°C is introduced. Thermally adiabatic boundary condition is specified at the side boundary. Also, temperature of particle and fluid is set 0 °C at the initial stage. The time step for both of the DEM and the thermal-fluid calculation is taken as 1.0x10⁻⁵ s.

Table 2 shows the material properties. The normal and shear stiffness for particle and wall are 1.0 x 10⁶ N/m. The friction coefficient for particle-particle contact is 0.5; also that for particle-wall is 0.3. The density of particles is 2650 kg/m³. Viscous damping without tensile force is used for energy dissipation at contacts. The ratio of the damping constant to the critical damping constant in the normal and shear direction is 0.05, which is equivalent to a restitution coefficient of 0.9. Thermal conductivity of particle assembly is 2.0 W/m.K and specific heat is 800 J/kg.K. Air is used as a fluid, with density and viscosity of 1.2 kg/m³ and 1.8e⁻⁵ Pa.s, respectively. Thermal conductivity and specific heat of air are 0.03 W/m.K and 1.0 kJ/kg.K respectively.

Figure 5: Model: particle assembly and fluid cell.
Table 2: Material properties.

<table>
<thead>
<tr>
<th>(Particle)</th>
<th>(Air)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number</td>
<td>2,400</td>
</tr>
<tr>
<td>Diameter</td>
<td>4mm</td>
</tr>
<tr>
<td>Density</td>
<td>2650 kg/m³</td>
</tr>
<tr>
<td>Viscosity</td>
<td>1.8e⁻⁵ Pa.s</td>
</tr>
<tr>
<td>Density</td>
<td>1.2 kg/m³</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>0.03 W/m.K</td>
</tr>
<tr>
<td>Normal Stiffness</td>
<td>1.0x10⁶ N/m</td>
</tr>
<tr>
<td>Shear stiffness</td>
<td>1.0x10⁶ N/m</td>
</tr>
<tr>
<td>Friction coefficient</td>
<td>0.5</td>
</tr>
<tr>
<td>Thermal Conductivity</td>
<td>2.0 W/m.K</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>800 J/kg.K</td>
</tr>
<tr>
<td>Coef. Of Linear Thermal Expansion</td>
<td>3.0x10⁻⁶ K⁻¹</td>
</tr>
</tbody>
</table>

(Wall)

| Normal Stiffness | 1.0x10⁶ N/m |
| Shear stiffness  | 1.0x10⁶ N/m |
| Friction coefficient | 0.3        |

Figure 6: General view; transient of particle temperature and fluid velocity vectors.

The simulation procedure is as follows. First, particles are created randomly within the rectangular space, then dropped by gravity. After reaching a steady-
state condition, air is injected at 2.6 m/s of apparent velocity from the center of bottom boundary for 5 seconds.

Figure 6 shows a general view and fluid velocity vectors for 5 seconds from the initial stage. Colour of each particle shows its temperature. The gas lifts particles near the injection point in the first stage. After that, particles migrate in the box, and the temperature of particles is gradually increased by forced convection and conduction heat transfer.

5 Summary

A particle-thermal-fluid coupling scheme with a mixed Lagrangian-Eulerian approach is developed by extending the author’s previous research. The scheme is described, with emphasis on the interaction term between particles and fluid. Two-dimensional simulations with forced convection heat transfer are conducted. As a result, it was found that thermal energy is exchanged correctly between particle and fluid. The scheme is believed to be useful for simulating coupled particle-thermal-fluid systems.

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References