CHAPTER V
MODELING AND SIMULATION TECHNIQUE

Mathematical simulation means the study of a system or its parts by manipulation of its mathematical representation or its physical model. The simulation has many benefits. It is possible to study existing system more quickly, economically and thoroughly than in the real system. Furthermore, with a suitable mathematical representation, it is possible to test extreme ranges of operating conditions, some of which might be impractical or unsafe to test in a real plant

A mathematical representation, namely mathematical model, is a mathematical abstraction of a real system. Model can be classified into three different categories, depending on how they are derived: first, theoretical models which are developed by using the principle of chemistry and physics, second, empirical models which are obtained from a mathematical (statistical) analysis of system data, and finally, models that compromise between the both categorized models with one or more parameters to be evaluated from plant data called semi-empirical models. In the last classification, certain theoretical model parameters such as heat transfer coefficient and similar fundamental relations usually must be evaluated from physical experiments or from process operating data.

In this chapter, a comprehensive model of heat transfer in two-dimensional spouted bed with draft plates using distinct element method is proposed. The model is derived from the model proposed by P.A. Cundall and O.D.L. Strack (1979) and T.B. Anderson and Jackson (1967). The heat transfer coefficient is estimated by Ranz-Marshall correlation (1952).

5.1 Model assumptions

The following assumptions are made in the modeling.

1. Gas is inviscid except for gas-particle vicinity.
2. Particles are assumed to be spherical and monodisperse.
3. Particles have a soft sphere interaction with a Hookian linear spring and a dash pot allowing multiple particle contacts under a Coulomb type friction condition.

4. Viscous damping effect is only indirectly included by taking into account inelastic collisions.
5. Particle-to-particle adhesion force and lubricating force are negligible.
6. Physical properties such as heat capacity, thermal conductivity, density and viscosity of gas and particles are assumed to be constant.
7. Heat loss through the vessel wall is neglected.
8. Temperature is uniform in each particle.
9. For the particle-to-gas heat transfer coefficient, the Ranz-Marshall correlation (1952) is applied for the local condition of each particle.
10. Direct particle-to-particle heat transfer is neglected.

5.2 Mathematical model

The present comprehensive mathematical model is based on the model proposed by P.A. Cundall and O.D.L. Strack (1979) and T.B. Anderson and R. Jackson (1967). The fluid motion is assumed two-dimensional and is solved simultaneously with the equation of motion of the particles by taking into account the interactions between the fluid and particles. The particle motion is calculated in three-dimensions by solving the Newton's equation of motion for each particle.

5.2.1 Continuous phase (gas phase)

The fluid motion follows the Navier Stokes eqation as follows:

Equation of continuity

$$\frac{\partial}{\partial t}\varepsilon + \frac{\partial}{\partial x_j}\left(\varepsilon u_j\right) = 0 \tag{5.1}$$

Equation of motion

$$\frac{\partial}{\partial t}\left(\varepsilon u_i\right) + \frac{\partial}{\partial x_j}\left(\varepsilon u_i u_j\right) = -\frac{\varepsilon}{\rho_g}\frac{\partial p}{\partial x_i} + f_{pi} \tag{5.2}$$

Fluid is treated as inviscid except the interaction term (f_{pi}) between the fluid and particles.

$$f_{pi} = \frac{\beta}{\rho_g}\left(\bar{v}_{pi} - u_i\right) \tag{5.3}$$

5.2.2 Disperse phase (solid phase)

The particle motion was calculated by solving the Newton's equation of motion for individual particle with taking into account gravity force (f_g), drag force (f_D) and contact force between the particles (f_C). The drag force is the sum of reaction force from Equation (5.3) and the pressure gradient as follows.

$$\boldsymbol{f}_D = \left(\frac{\beta}{1-\varepsilon}\left(\boldsymbol{u} - \boldsymbol{v}_p\right) - \frac{\partial p}{\partial x}\right)V_p \tag{5.4}$$

where V_p is the volume of a particle. The contact force is calculated by using the DEM proposed by Cundall and Strack (1979). A particle often contacts with many particles or walls. Therefore, the contact force f_C is the sum of all these contact forces. The Newton's equation of motion can be written as follows:

$$\ddot{\boldsymbol{x}} = \frac{\boldsymbol{f}_C + \boldsymbol{f}_D}{m} + \boldsymbol{g} \tag{5.5}$$

where m is the mass of a particle. The rotational motion of a particle caused by tangential force is derived from

$$\dot{\boldsymbol{\omega}} = \frac{\boldsymbol{T}}{I} \tag{5.6}$$

where T is the torque caused by the tangential components of the contact forces. I is the moment of inertia of a particle.

5.3 Complementary equations

5.3.1 Continuous phase (gas phase)

Equation of energy was derived from C.Crowe, M. Sommerfeld and Y.Tsuji (1998). The detail are shown in Appendix A and B. The final equation is as follow:

$$\frac{\partial}{\partial t}\left(\varepsilon T_g\right)+\frac{\partial}{\partial x_i}\left(\varepsilon u_i T_g\right)=\frac{Q_s}{\rho_g c_{p,g}}+\frac{1}{\rho_g c_{p,g}}\frac{\partial}{\partial x_i}\left(k_c\frac{\partial T_g}{\partial x_i}\right) \tag{5.7}$$

$$Q_s=\frac{6(1-\varepsilon)}{d_{p,k}}\left\langle h_d\left(T_{p,k}-T_g\right)\right\rangle$$

Well-known correlations of heat transfer for an individual spherical particle have been proposed by W.E. Ranz and W.R. Marshall (1952). The correlations are

$$Nu=2.0+0.6\,\mathrm{Pr}^{1/3}\,\mathrm{Re}^{1/2} \tag{5.8}$$

where

$$Nu = h_p d_p / k_c$$

$$Pr = c_{p,g}\mu_g / k_c$$

$$Re=\frac{\left|\bar{\boldsymbol{v}}_p-\boldsymbol{u}\right|\rho_g\varepsilon d_p}{\mu_g}$$

Q_s is the heat transfer rate between a particle and gas in a unit volume. k_c and $c_{p,g}$ are the thermal conductivity of gas and heat capacity of gas respectively.

5.3.2 Disperse phase (solid phase)

$$\begin{Bmatrix}\text{Rate of accumulation} \\ \text{of energy of a particle}\end{Bmatrix} = \begin{Bmatrix}\text{Rate of heat transfer} \\ \text{from gas phase}\end{Bmatrix}$$

$$\rho_p c_{p,g} V_{p,k} \frac{dT_{p,k}}{dt} = -h_p A_{p,k}\left(T_{p,k} - T_g\right) \tag{5.9}$$

where $V_{p,,k}$ is the volume of a particle. $c_{p,g}$ and $A_{p,k}$ is the specific heat of a particle and external surface area of a particle.

5.4 Boundary condition

Array of numerical grids of fluid motion is shown in Figure 5.1.

I.C.: at $t = 0$, $v_y = 0$, for all fluid cell $v_z = 0$, for all fluid cell

$T_d = T_{pi}$, for all particle $T_g = T_{gi}$, for all fluid cell

The injected gas

B.C.: at $t > 0$,

$v_y(7,0) = 0$, $v_y(9,0) = 0$

$v_y(10,0) = 0$, $v_y(8,0) = v_y(8,1)$

$v_z(8,0) = 8u/\varepsilon(8,1)$, $v_z(9,0) = 8u/\varepsilon(9,1)$

$T_g(8,0) = T_i$, $T_g(9,0) = T_i$

$T_g(7,0) = T_g(7,1)$, $T_g(10,0) = T_g(10,1)$

An outflow boundary

B.C.: at $t > 0$,

$v_y(i,j_{max}) = v_y(i,j_{max}+1)$

$v_z(i,j_{max}) = v_z(i,j_{max}+1)$

$T_g(i,j_{max}) = T_g(i,j_{max}+1)$

A sidewall (a slip wall condition)

B.C.: at $t > 0$

$v_y(0, j) = 0$ (for $j \geq 8$)

$v_z(0, j) = v_z(1, j)$ (for $j \geq 8$)

$v_y(16, j) = 0$ (for $j \geq 8$)

$v_z(17, j) = v_z(16, j)$ (for $j \geq 8$)

$T_g(0, j) = T_g(1, j)$ (for $j \geq 8$)

$T_g(17, j) = T_g(16, j)$ (for $j \geq 8$)

A taper wall

B.C.: at $t > 0$

$v_y(j-1, 8-j) = 0$ (for $1 \leq j \leq 7$)

$v_z(j-1, 8-j) = 0$ (for $1 \leq j \leq 7$)

$v_y(9+j, j) = 0$ (for $1 \leq j \leq 7$)

$v_z(10+j, j) = 0$ (for $1 \leq j \leq 7$)

$T_g(j-1, 8-j) = T_g(j, 8-j)$ (for $1 \leq j \leq 7$)

$T_g(10+j, j) = T_g(9+j, j)$ (for $1 \leq j \leq 7$)

The draft plates (a slip wall condition, no thickness and insulate)

B.C.: at $t > 0$

$v_y(6, j) = 0$ (for $5 \leq j \leq 14$)

$v_z(7, j) = v_z(6, j)$ (for $1 \leq i \leq 6$, $5 \leq j \leq 14$)

$v_z(6, j) = v_z(7, j)$ (for $7 \leq i \leq 10$, $5 \leq j \leq 14$)

$T_g(7, j) = T_g(6, j)$ (for $1 \leq i \leq 6$, $5 \leq j \leq 14$)

$T_g(6, j) = T_g(7, j)$ (for $7 \leq i \leq 10$, $5 \leq j \leq 14$)

$v_y(10, j) = 0$ (for $5 \leq j \leq 14$)

$v_z(11, j) = v_z(10, j)$ (for $7 \leq i \leq 10$, $5 \leq j \leq 14$)

$v_z(10, j) = v_z(11, j)$ (for $10 \leq i \leq 16$, $5 \leq j \leq 14$)

$T_g(11, j) = T_g(10, j)$ (for $7 \leq i \leq 10$, $5 \leq j \leq 14$)

$T_g(10, j) = T_g(11, j)$ (for $10 \leq i \leq 16$, $5 \leq j \leq 14$)

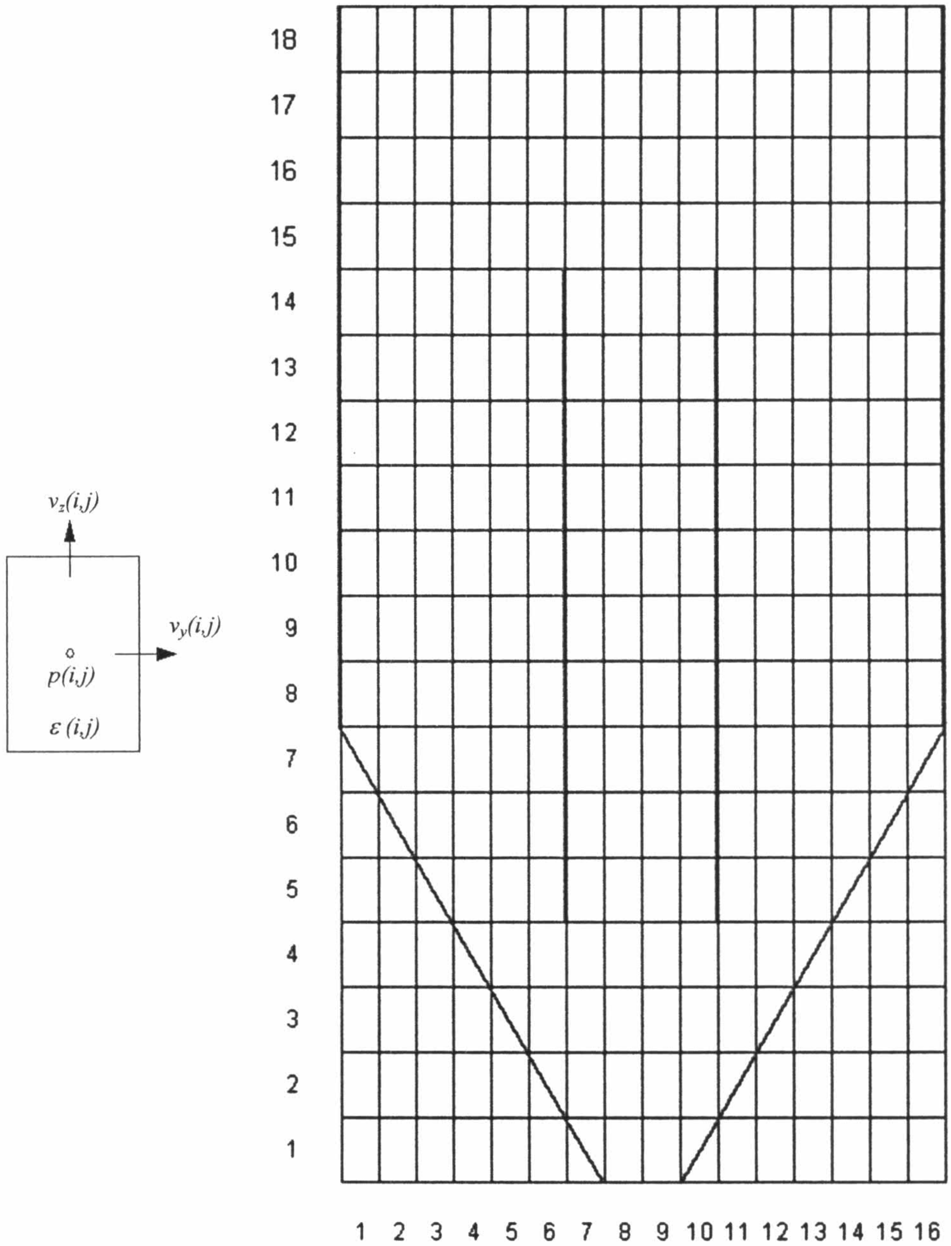

Figure 5.1 Array of numerical grids of fluid motion

5.5 Simulation Technique

5.5.1 Input data

The data required in the simulation are listed as follows:

1. Vessel configuration: width, depth and height of vessel.
2. Cell size of fluid motion: width and height.
3. Grid size of particle: width, depth and height.
4. Physical properties of particle: diameter, density, spring constant, coefficient of restitution, coefficient of friction, poisson's ratio, specific heat and number of particle.
5. Physical properties of air: density, viscosity, specific heat and thermal conductivity.
6. Inlet conditions: air and particle temperature and inlet air temperature
7. Model parameters: Maximum possible number of contacting particles, integration time step interval, total number of integration steps and relaxation factor.

It should be noted that the spring constant has been assumed for convenience of the calculation.

5.5.2 Numerical approach

Finite difference methods used to solve partial differential equations (PDE) in this model. In these methods, the solution domain is divided into a grid of discrete points or nodes. The PDE is then written for each node and its derivatives replaced by finite divided differences. Semi-Implicit Method for Pressure-Linked Equation (SIMPLE) method has been carried out to solve PDE in this model.

5.5.3 Algorithm of heat transfer in the spouted bed with draft plates

A simplified algorithm of this model is listed below. Figure 5.2 illustrates the simplified flow chart of the model.

1. Input all the data mentioned in section 5.4.1.
2. Calculate void fraction in each fluid cell in the vessel.

3. Set boundary condition of fluid cell and determine particle grids used for checking possible particle contacts.
4. Calculate fluid motion by using SIMPLE method as mentioned in section 5.4.3.
5. Calculate particle motion by solving the Newton's equation of motion for individual particle with taking into account gravity force, drag force and contact force between the particles.
6. Calculate fluid temperature by solving equation of energy in section 5.3.1 with p, u and v from step 4.
7. Calculate particle temperature mentioned in section 5.3.2.
8. Check integration time step interval
9. Write the results to file.

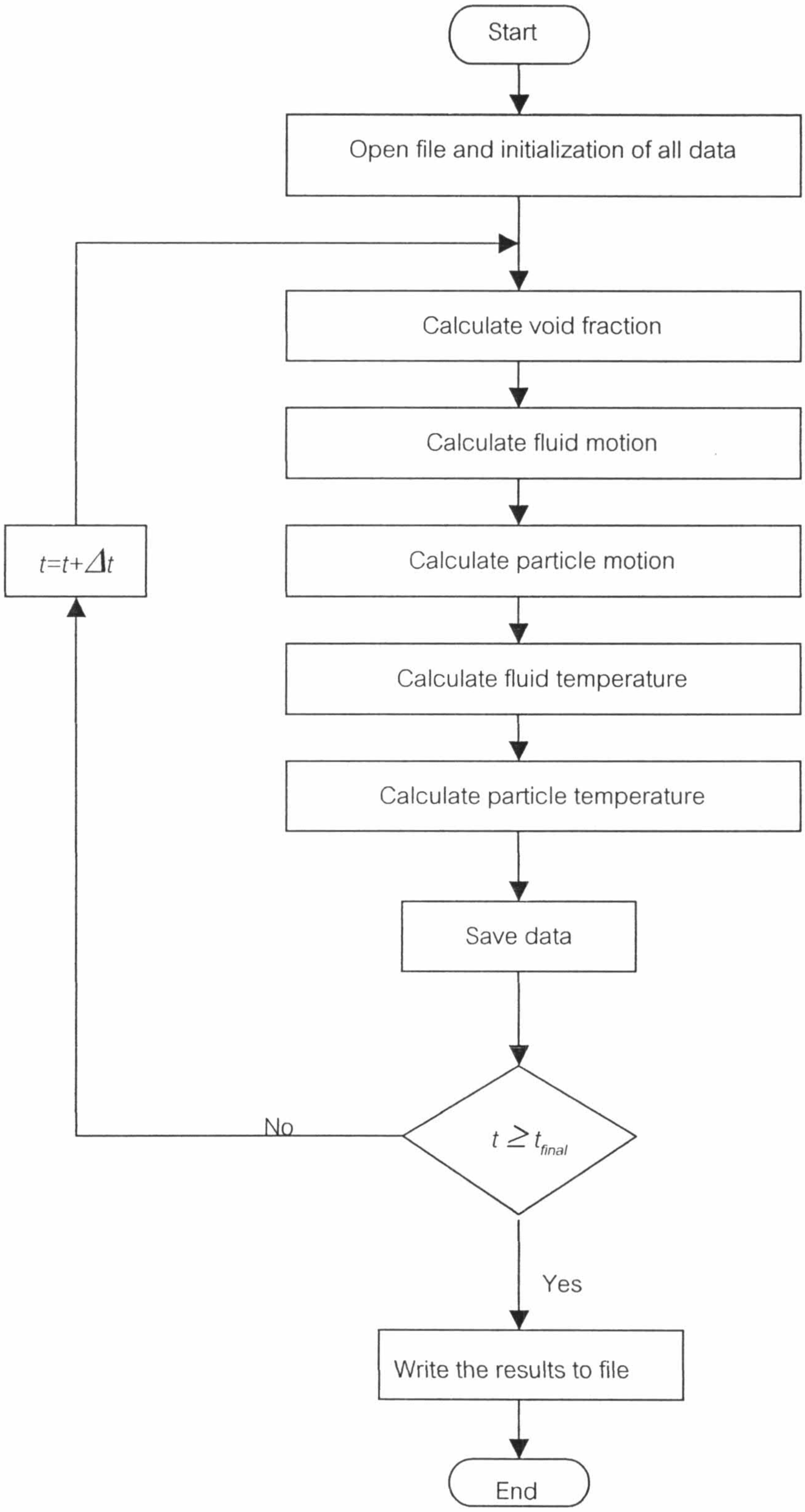

Figure 5.2 Block diagram of heat transfer in spouted bed with draft plates