

CHAPTER IV SIMULATION



4.1 Simulation System

This simulation used IIT code in Fortran language. This IIT code composed of IIT hydrodynamic models and computer code, which the fundamental of hydrodynamics was explained on “Multiphase Flow and Fluidization, Continuum and Kinetic Theory Descriptions” by Dimitri Gidaspow (1994). This program could use model A and model B in Gidaspow’s book (1994) and calculate the pressure drop in the continuous phase. The model B was unconditionally well posed, which was different from model A. For this experiment, it was found that the velocity of the glass beads and Reynolds stresses in the bubble. It found the bubble size and the bubble velocity as well. These data would be compared with the IIT hydrodynamic model.

The physical properties and the operative condition were shown in table 4.1. Input data on ‘sam.d1’ file in simulation had many variable as shown in table 4.2. “examp1.r” was the name of the restart file. Data were saved regularly in this file. “sample input data file for Che 536 Project” was the title of the problem. “gas.out” and “solid.out” were the output file for fluid volume fraction and solid volume fraction, respectively. “ratio” was separation ratio but it was not used in the simulation. The coordinate system was set by ITC variable (0=Cartesian, and 1=Cylindrical) and the number of cells in x- and y- direction were defined by IB2 and JB2, respectively. But the mesh size in x- and y- direction were defined by DR (I) and DZ(J), respectively. The means of these input parameters were explained in appendix B. The number of line at NSO=1, 5, and 7 is equaled to the value of NFL, NIN, and NOUT, respectively. For DK(K), RL(K), PHI(K), CPHI(K), PVISC(K), UIO(K,N), VIO(K,N), PIO(K), THIO(K,N), and TEMIO(K,N), if K is equaled to 0, these parameters are the parameters of fluid. On the other hand, if K is not equaled to 0, these parameters are the parameters of solid.

Table 4.1 Geometry physical properties, and operative conditions in simulation

Detail	Value
Width of the fluidized bed	15.4 cm
Depth of the fluidized bed	2.2 cm
Height of the initial packed bed	14.5 cm
Total height of the fluidized bed	58.5 cm
Superficial gas velocity	68.5 cm
Temperature	300 K
Pressure at bottom	1.042 atm
Gas	Air
Solid	Glass bead particle
Size of solid	530 micron
Density of solid	2.50 g/cm ³
Grid size (dx * dy)	many grid size
Number of cells in the grid	30 * 75
Time interval	10 ⁻⁵ sec

Table 4.2 Input data on 'sam.d1' file in simulation program

Descriptions	Input Data
REFILE: Restart file name	Examp1.r
NAME: Problem identifier	Input data file for glass beads 530 microns
GAS: Fluid phase concentration output file name	Gas.out
SOLID: Solid phase concentration output file name	Solid.out

Descriptions	Input Data
RATIO: Mass withdraw ration and quality ratio output file name	Ratio
ITC, IB2, JB2, NSOLID	0 30 75 1
RST	0.0
DR(I), I=1 to IB2	0.6 28*0.55 0.6
DZ(J), J=1 to JB2	0.6 30*0.475 6*0.55 2*0.60 2*0.65 5*0.75 2*0.8 2*0.9 5*1.1 20*1.29
NCONT, MODAB, IPRES, ICOH, ISWIT, IFLZB	1 2 1 0 0 1
DK(0), RL(0), PHI(0), CPHI(0), PVISC(0) (applied for fluid phase)	0.4 1.206E-03 1.0 1.0 1.82E-04
DK(1), RL(1), PHI(1), CPHI(1), PVISC(1) (applied for solid phase)	0.0530 2.50 1.0 0.6413 1.0
NSL(M), M=1 to 4	3 3 3 3
NFL, NIN, NOUT, NOBS	2 5 1 0
NSO(1), (IOB(M,1), M=1 to 4)	1 2 29 31 74
2 2	1 2 29 2 30
3 3	5 3 3 1 1
4 4	5 4 4 1 1
5 5	5 5 26 1 1

Descriptions		Input Data				
6	6	5	27	27	1	1
7	7	5	28	28	1	1
8	8	5	3	28	75	75
UIO(0,1), VIO(0,1), PIO(0,1), THIO(0,1), TEMIO(0,1) (fluid phase)		0.0	0.0	1.01325E+06	1.0	300.0
UIO(1,1), VIO(1,1), PIO(1,1), THIO(1,1), TEMIO(1,1) (solid phase)		0.0	0.0	0.0	0.0	
UIO(0,2), VIO(0,2), PIO(0,2), THIO(0,2), TEMIO(0,2) (fluid phase)		0.0	20	1.01325E+06	0.49	300.0
UIO(1,2), VIO(1,2), PIO(1,2), THIO(1,2), TEMIO(1,2) (solid phase)		0.0	0.0	0.51	300.0	
UIO(0,3), VIO(0,3), PIO(0,3), THIO(0,3), TEMIO(0,3) (fluid phase)		0.0	22.9	1.042E+06	1.0	300.0
UIO(1,3), VIO(1,3), PIO(1,3), THIO(1,3), TEMIO(1,3) (solid phase)		0.0	0.0	0.0	300.0	
UIO(0,4), VIO(0,4), PIO(0,4), THIO(0,4), TEMIO(0,4) (fluid phase)		0.0	45.8	1.042E+06	1.0	300.0
UIO(1,4), VIO(1,4), PIO(1,4), THIO(1,4), TEMIO(1,4) (solid phase)		0.0	0.0	0.0	300.0	
UIO(0,5), VIO(0,5), PIO(0,5), THIO(0,5), TEMIO(0,5) (fluid phase)		0.0	68.5	1.042E+06	1.0	300.0
UIO(1,5), VIO(1,5), PIO(1,5), THIO(1,5), TEMIO(1,5) (solid phase)		0.0	0.0	0.0	300.0	
UIO(0,6), VIO(0,6), PIO(0,6), THIO(0,6), TEMIO(0,6) (fluid phase)		0.0	45.8	1.042E+06	1.0	300.0
UIO(1,6), VIO(1,6), PIO(1,6), THIO(1,6), TEMIO(1,6) (solid phase)		0.0	0.0	0.0	300.0	
UIO(0,7), VIO(0,7), PIO(0,7), THIO(0,7), TEMIO(0,7) (fluid phase)		0.0	22.9	1.042E+06	1.0	300.0

Descriptions	Input Data
UIO(1,7),VIO(1,7), PIO(1,7), THIO(1,7), TEMIO(1,7) (solid phase)	0.0 0.0 0.0 300.0
UIO(0,8),VIO(0,8), PIO(0,8), THIO(0,8), TEMIO(0,8) (fluid phase)	0.0 0.0 1.01325E+06 1.0 300.0
UIO(1,8),VIO(1,8), PIO(1,8), THIO(1,8), TEMIO(1,8) (solid phase)	0.0 0.0 0.0 300.0
ITD (switch on restarting the program)	0
TIME, TSTOP, DT, ITX	0.0 1.0 0.00001 1
TPR, TDUMP, TPRR	0.01 0.01 1.0
ITXMX, (DTNXT(IX), IX=1 to ITXMX)	1 0.00001
GRAVX, GRAVY	0.0 -980.621
EPSG, THMIN, RLIM, ISTW	1.0E-05 0.3587 1.0E-05 0
NIMBR, LCAT1, LCAT2	1 51 39

A diagram of grid lines on this simulation was shown in figure 4.1.

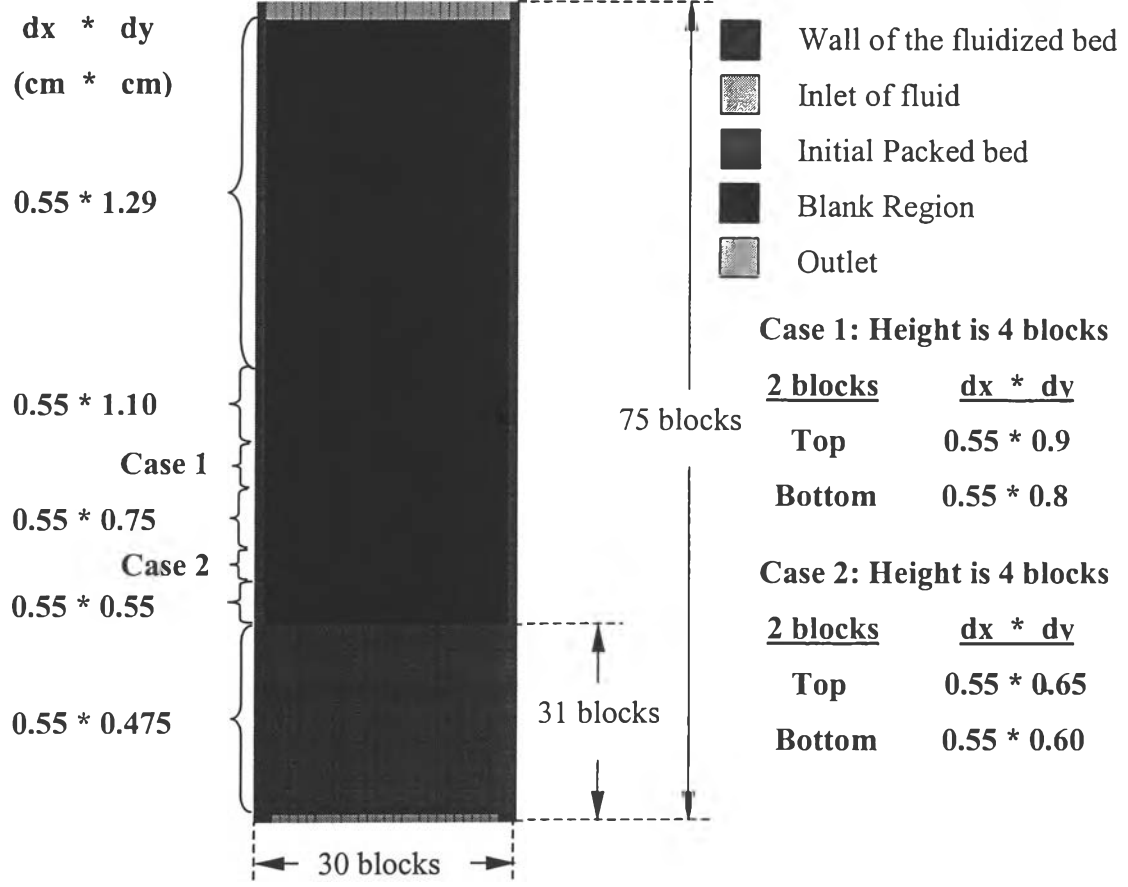


Figure 4.1 A schematic diagram of the simulation in two dimensional fluidized beds.

4.2 Methodology

4.2.1 Boundary Conditions

The rectangular region was partitioned into cells of sizes δx_i in x-direction and δz_i in y-direction. A perimeter of fictitious (dummy) boundary cells surrounding the computing mesh was used to enforce boundary conditions. Several boundary conditions were programmed in the code around the computing mesh perimeter. The cell flag types were indicated by IFL(I,J).

<u>Flag</u>	<u>Cell Type</u>
1	Fluid Cell
2	Free-slip rigid walls
3	No-slip rigid walls for gas/liquid phases
4	Continuative outflow
5	Prescribed inflow rate
6	Prescribed pressure inflow
7	Prescribed pressure outflow with particulate outflow
8	Prescribed pressure outflow with no particulate outflow

In the bottom row and left column of boundary cells, flag types 5 and 6 could specify inflow. Boundaries represented rigid cells or wall cells might define flag types 2 and 3. Obstacle blocks within the computing mesh were built from rigid cells, flag types (IFL = 2 or 3) as shown in figure 5.2.

The position of all blocks had to match with rectangular cells within the computing mesh. Calculations were not performed in the obstacle cells, only in the remaining fluid cells within the computing mesh. Cell flag type (IFL = 1) was a computational cell.

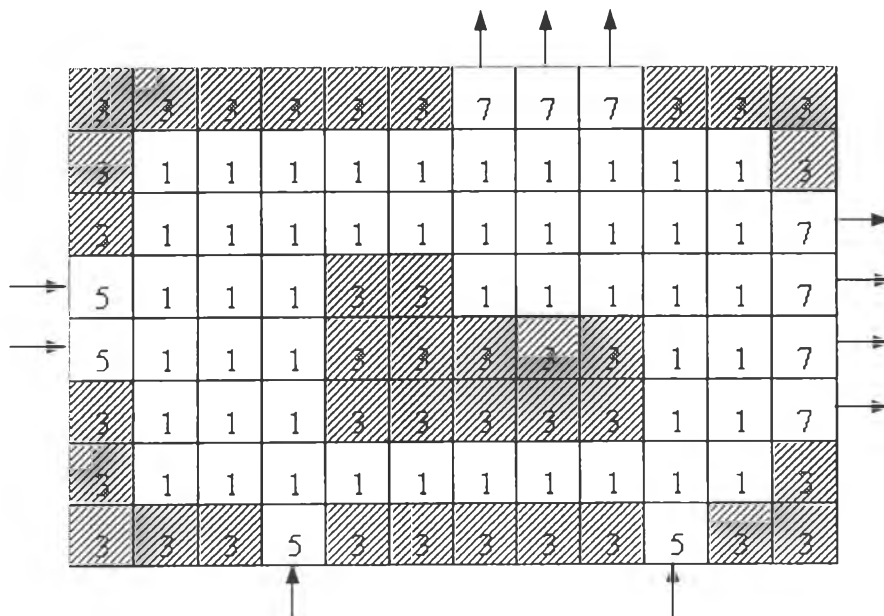


Figure 4.2 Boundary centered variables in a fluid cell of the computational mesh.

4.2.2 Rigid Cells

A rigid (solid) cell might specify three types of boundary conditions: free-slip, no-slip or partial slip (IFL = 2 or 3). The partial slip boundary was applied for only solid phases. A free-slip boundary in two dimensions was represented line of symmetry. A non-adhering boundary exerted no drag on the fluid and a no-slip boundary represents a viscous boundary exerted a drag on the fluid. If cell (i,j) was considered to a fluid cell, an inflow boundary cell, or an outflow boundary cell. An adiabatic rigid cell was a corner cell, if it had at least two adjacent edges. Each edge was shared with a fluid cell, an inflow boundary cell, or an outflow boundary cell.

If right cell (i+1,j) or left cell (i-1,j), was a rigid cell, then for all time levels n,

$$(u_k)_{i\pm\frac{1}{2},j}^{n+1} = 0 \quad (4.1)$$

$$(v_k)_{i\pm 1,j+\frac{1}{2}}^{n+1} = \begin{cases} (v_k)_{i,j+\frac{1}{2}}^n & \text{for (IFL = 2)} \\ -\delta r_{i\pm 1} (v_k)_{i,j+\frac{1}{2}}^n / \delta r_i & \text{for (IFL = 3), } k \neq \text{solid} \\ \left(\frac{2\lambda_{i,j} - \delta r_{i\pm 1}}{2\lambda_{i,j} - \delta r_i} \right) (v_k)_{i,j+\frac{1}{2}} & \text{for (IFL = 3), } k = \text{solid} \end{cases} \quad (4.2)$$

Correspondingly, if top cell (i,j+1) or bottom cell (i,j-1), was a rigid cell, free-slip boundary conditions (IFL = 2) or no-slip boundary conditions (IFL = 3) were ordered, then for all n,

$$(v_k)_{i,j\pm\frac{1}{2}}^{n+1} = 0 \quad (4.3)$$

$$(u_k)_{i\pm 1, j+\frac{1}{2}}^{n+1} = \begin{cases} (u_k)_{i+\frac{1}{2}, j}^n & \text{for (IFL = 2)} \\ -\delta z_{i\pm 1} (u_k)_{i+\frac{1}{2}, j}^n / \delta z_i & \text{for (IFL = 3), } k \neq \text{solid} \\ \left(\frac{2\lambda_{i,j} - \delta z_{j\pm 1}}{2\lambda_{i,j} - \delta z_j} \right) (u_k)_{i+\frac{1}{2}, j} & \text{for (IFL = 3), } k = \text{solid} \end{cases} \quad (4.4)$$

If any one of the cells $(i, j+1)$, $(i+1, j)$, $(i-1, j)$, or $(i, j-1)$ was both a rigid cell and a corner cell, the velocities of components located at the center for free slip, no slip and partial slip boundary conditions were equaled to zero.

4.2.3 Inflow Boundary Cells

The input data had to define a pressure (p_f), velocities and volume fractions, ϵ_k for all phases ($k = f, 1, 2, \dots, N$; $k=f$ for fluid phase and $k \geq 1$ for solid phases). The inflow boundary conditions had 2 types: inflow composed of flow rate and pressure (IFL=5), and inflow pressure (IFL=6). Both types required pressure to calculate the mass fluxes, but the momentum equations were used to find the radial or axial velocity of components, when the inflow pressure was prescribed.

4.2.4 Outflow Boundary Cells

For outflow boundary conditions, the input data had to define the pressure, and the tangential velocity was equaled to zero. Outflow boundary conditions had 2 types: pressure prescribed outflow with particulate outflow (IFL = 7), or no particulate outflow (IFL = 8); or continuative outflow (IFL = 4). Therefore, the type for IFL=8 did not have particle leaving from the fluidized bed. For all types, reflection could give the volume fractions to outflow cells, while this program was running.

Therefore, the top outflow boundary had $(i, j) = (I, JB2)$; $(i+1/2, j) = (I, JB2)$; $(i, j+1/2) = (I, JB2)$; $(i, j-1) = (I, JB1)$; and $(i, j-1/2) = (I, JB1)$,

$$(p_f)_{i,j}^{n+1} = \begin{cases} p_0 & \text{for (IFL = 7 or 8)} \\ (p_f)_{i,j-1}^n & \text{for (IFL = 4).} \end{cases} \quad (4.5)$$

$$(\varepsilon_k)_{i,j}^{n+1} = \begin{cases} (\varepsilon_k)_{i,j-1}^n & \text{for (IFL = 4 or 7).} \\ 1 & \text{for (IFL = 8), } k=f \\ 0 & \text{for (IFL = 8), } k \neq f \end{cases} \quad (4.6)$$

$$(u_k)_{i+\frac{1}{2},j}^{n+1} = 0 \quad (4.7)$$

$$(v_k)_{i,j+\frac{1}{2}}^{n+1} = (\varepsilon_f \rho_f)_{i,j-1}^{n+1} (v_f)_{i,j-\frac{1}{2}}^{n+1} / (\varepsilon_f \rho_f)_{i,j}^{n+1} \quad (4.8)$$

$$(v_k)_{i,j+\frac{1}{2}}^{n+1} = \begin{cases} (\varepsilon_k \rho_k)_{i,j-1}^{n+1} (v_k)_{i,j-\frac{1}{2}}^{n+1} / (\varepsilon_k \rho_k)_{i,j}^{n+1} & \text{for (IFL = 4 or 7)} \\ 0 & \text{for (IFL = 0).} \end{cases} \quad (4.9)$$

The right outflow boundary had $(i,j) = (IB2,J)$; $(i+1/2,j) = (IB2,J)$; $(i-1,j) = (IB1,J)$; and $(i-1/2,j) = (IB1,J)$.

$$(p_f)_{i,j}^{n+1} = \begin{cases} p_0 & \text{for (IFL = 7 or 8).} \\ (p_f)_{i-1,j}^n & \text{for (IFL = 4).} \end{cases} \quad (4.10)$$

$$(\varepsilon_k)_{i,j}^{n+1} = \begin{cases} (\varepsilon_k)_{i-1,j}^n & \text{for (IFL = 4 or 7).} \\ 1 & \text{for (IFL = 8), } k=f \\ 0 & \text{for (IFL = 8), } k \neq f \end{cases} \quad (4.11)$$

$$(v_k)_{i,j+\frac{1}{2}}^{n+1} = 0 \quad (4.12)$$

$$(u_f)_{i+\frac{1}{2},j}^{n+1} = r_{i-\frac{1}{2}} (\varepsilon_f \rho_f)_{i-1,j}^{n+1} (u_f)_{i-\frac{1}{2},j}^{n+1} / \left[r_{i+\frac{1}{2}} (\varepsilon_f \rho_f)_{i,j}^{n+1} \right] \quad (4.13)$$

$$(u_k)_{i+\frac{1}{2},j}^{n+1} = \begin{cases} r_{i-\frac{1}{2}} (\varepsilon_k \rho_k)_{i-1,j}^{n+1} (u_k)_{i-\frac{1}{2},j}^{n+1} / \left[r_{i+\frac{1}{2}} (\varepsilon_k \rho_k)_{i,j}^{n+1} \right] & \text{for (IFL = 4 or 7).} \\ 0 & \text{for (IFL = 0).} \end{cases} \quad (4.14)$$

4.2.5 Initial Conditions

The simulation beginning had to be the initial condition specified all fields of variables. The input data would define that inflow was uniform or non-uniform velocity profile. The blocks which fluid could flow will specify the type of IFL=1. The pressure in the axial direction was initialized by the gravity of the fluid and particulate phases over that position. But If IPRES was equaled to zero, pressure profile was obtained by using fluid phase only and the fluid phase did not support the weight of the particulate phases. On the other hand, if IPRES was equaled to one, the fluid phase supported the weight of the complete bed. The pressure distribution in all fluid cells was computed recursively from the weight of the bed as follows,

$$(p_f)_{i,j} = (p_f)_{i+1,j} - g_z \delta_{z,j+\frac{1}{2}}^* \left\{ \begin{array}{ll} (\epsilon_f \rho_f)_{i,j+\frac{1}{2}} & \text{for (IPRES = 0).} \\ \sum_{k=f,1}^N [(\epsilon_k \rho_k)_{i,j+\frac{1}{2}}] & \text{for (IPRES = 1)} \end{array} \right. \quad (4.15)$$

where pressure in the most top cell $J = JB2$ was given by $(p_f)_{i,j+1/2} = p_0$. For density of fluid, equation of state or any equivalent relation might be used. Since this density might depend on the pressure in cell (i,j) which was yet to be calculated, a quadratic equation had to be solved.