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Letter to the Editor

Two-dimensional discrete particle model: Comment on the numerical simulation of cluster flow behavior in the riser of circulating fluidized beds by Liu and Lu

In a recent paper, Liu and Lu [1] reported the results of a numerical study on the cluster flow behavior in the riser of circulating fluidized beds using a two-dimensional discrete particle model (2D-DPM). Below we discuss the severe shortcomings of the phase coupling scheme used in the context of a two-dimensional DPM.

The 2D-DPM has been widely used to study the gas–solid flow behavior in fluidized bed since it was first introduced by Tsuji et al. [2] for the soft-sphere version and Hoomans et al. [3] for the hardsphere approach. When a finite volume method is applied, the local 2D voidage ε_{2D} can be calculated based on the space or area occupied by the particles in the 2D grid cells. This is not consistent with the empirical drag formula in which the correlated porosity ε_{3D} is evaluated based on real 3D systems. To correct this inconsistency, two strategies are often used to transform the 2D porosity. The first one was suggested by Hoomans et al. [3] and it is described by the following equation:

$$\varepsilon_{3D} = 1 - \frac{2}{\sqrt{\pi\sqrt{3}}} (1 - \varepsilon_{2D})^{3/2}$$
 (1)

This equation is derived on the basis of a comparison between a 2D hexagonal lattice and a 3D cubic lattice assuming equal interparticle distances. The second strategy was presented by Xu and Yu [4], in which the 2D domain is regarded as a pseudo 3D one with a thickness of one particle diameter.

Liu and Lu [1] have opted for the first strategy. In this work, the source term due to particle drag in the gas momentum equations was evaluated using the following equation (Eq. (5) in [1])

$$S_{p-g} = \frac{\sum_{i=1}^{N} f_{d,i}}{s} \tag{2}$$

N is the number of particles in the area *s*. Similar formula can also be found in their earlier publications [5-8]. This formula ensures that the interaction forces between the two phases are equal and have reverse directions as stated in [1,5-7]. However this scheme underpredicts the momentum source term, which results in a much lower prediction of the pressure drop of the fluidized bed and erroneous prediction of the minimum fluidization velocity. This can be demonstrated if we consider a 2D stagnant bed at the incipient fluidization state. Since the particles are homogeneously distributed in the bed without any motion, the gas flow is steady and the gradients of the static pressure are constant. The gas momentum equation (Eq. (2) in [1]) in the vertical direction is reduced to

$$-\varepsilon_g \frac{\partial p}{\partial y} - S_{p-g} - \varepsilon_g \rho_g g = 0 \tag{3}$$

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Applying the finite volume method, integration of the above equation over a 2D grid cell reads

$$-\varepsilon_g \frac{\partial p}{\partial y} \Delta x \Delta y - \sum_{i=1}^{Nc} f_{d,i} - \Delta x \Delta y \varepsilon_g \rho_g g = 0$$
(4)

where *Nc* is the number of particles in the cell. The particle momentum equation (Eq. (7) in [1]) is reduced to

$$-\frac{\pi}{6}d_i^3\frac{\partial p}{\partial y} + f_{d,i} - m_i g = 0$$
⁽⁵⁾

Summation over all particles in the cell reads

$$-\frac{\pi}{6}\frac{\partial p}{\partial y}\sum_{i=1}^{Nc}d_{i}^{3} + \sum_{i=1}^{Nc}f_{d,i} - g\sum_{i=1}^{Nc}m_{i} = 0$$
(6)

The addition of Eqs. (4) and (6) yields

$$-\frac{\partial p}{\partial y} = \left(\frac{\pi \sum_{i=1}^{Nc} d_i^3}{\pi \sum_{i=1}^{Nc} d_i^3 + 6\varepsilon_g \Delta x \Delta y}\right) \rho_p g + \left(\frac{6\varepsilon_g \Delta x \Delta y}{\pi \sum_{i=1}^{Nc} d_i^3 + 6\varepsilon_g \Delta x \Delta y}\right) \rho_g g$$
(7)

It is well known that the pressure drop across a stagnant bed at the incipient fluidization state is equal to the weight of the bed. Thus the pressure gradient reads as

$$-\frac{\partial p}{\partial y} = (1 - \varepsilon_g)\rho_p g + \varepsilon_g \rho_g g \tag{8}$$

It is very easy to prove that the pressure drop estimated by Eq. (7) is much less than that computed using Eq. (8). This is true whether the void fraction ε_g is calculated by Eq. (1) or when it is taken equal to ε_{2D} , given that the particle size should be always smaller than the cell size for DPM calculations. Thus the two-phase coupling scheme presented by Liu and Lu [1] yields an extremely under-predicted pressure drop, and thus an erroneous prediction of the minimum fluidization velocity. Actually Eq. (7) is equivalent to Eq. (8) only when the void fraction is evaluated by

$$\varepsilon_g = 1 - \frac{\pi \sum_i^{Nc} d_i^3}{6\Delta x \Delta y} \tag{9}$$

Obviously formula (9) over-predicts the void fraction compared to its exact value for a 3D system. Since the pressure gradient force plays a very important role in the two- phase motion, the two-phase coupling scheme presented in [1,5–8] may cause an inaccurate analysis of the gas-particle flow behavior in the circulating fluidized bed riser.

References

- H. Liu, H. Lu, Numerical study on the cluster flow behavior in the riser of circulating fluidized beds, Chemical Engineering Journal 150 (2009) 374–384.
- [2] Y. Tsuji, T. Kawaguchi, T. Tanaka, Discrete particle simulation of two-dimensional fluidized bed, Powder Technology 77 (1993) 79–87.
- [3] B.P.B. Hoomans, J.A.M. Kuipers, W.J. Briels, W.P.M. van Swaaij, Discrete particle simulation of bubble and slug formation in a two-dimensional gas-fluidised bed: a hard-sphere approach, Chemical Engineering Science 51 (1996) 99–118.
- [4] B.H. Xu, A.B. Yu, Numerical simulation of the gas–solid flow in a fluidized bed by combining discrete particle method with computational fluid dynamics, Chemical Engineering Science 52 (1997) 2785–2809.
- [5] S. Wang, X. Li, H. Lu, L. Yu, J. Ding, Z. Yang, DSMC prediction of granular temperatures of clusters and dispersed particles in a riser, Powder Technology 192 (2009) 225–233.
- [6] S. Wang, H. Liu, H. Lu, W. Liu, J. Ding, W. Li, Flow behavior of clusters in a riser simulated by direct simulation Monte-Carlo method, Chemical Engineering Journal 106 (2005) 197–211.
- [7] H. Lu, Z. Shen, J. Ding, X. Li, H. Liu, Numerical simulation of bubble and particles motions in a bubbling fluidized bed using direct simulation Monte-Carlo method, Powder Technology 169 (2006) 159–171.

[8] H. Lu, S. Wang, Y. Zhao, Y. Liu, D. Gidaspow, J. Ding, Prediction of particle motion in a two-dimensional bubbling fluidized bed using discrete hard-sphere model, Chemical Engineering Science 60 (2005) 3217–3231.

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