DISCRETE PARTICLE SIMULATION OF DENSE PHASE PARTICULATE FLOWS

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First, methods of numerical analysis of gas-particle flows is classified into micro, meso and macro scale approaches based on the concept of multi-scale mechanics. Next, the explanation moves on to discrete particle simulation where motion of individual particles is calculated numerically using the Newtonian equations of motion. The author focuses on the cases where particle-to-particle interaction has significant effects on the phenomena. Concerning the particle-to-particle interaction, two cases are considered: the one is collision-dominated flows and the other is the contact-dominated flows. To treat this interaction mathematically, techniques named DEM(Distinct Element Method) or DSMC (Direct Simulation Monte Carlo) have been developed. DEM, which has been developed in the field of soil mechanics, is useful for the contact -dominated flows and DSMC method, developed in molecular gas flows, is for the collision-dominated flows. Combining DEM or DSMC with CFD (computer fluid dynamics), the discrete particle simulation becomes a more practical tool for industrial flows because not only the particle-particle interaction but particle-fluid interaction can be handled. As examples of simulations, various results are shown, such as hopper flows, particle segregation phenomena, particle mixing in a rotating drum, dense phase pneumatic conveying, spouted bed, dense phase fluidized bed, fast circulating fluidized bed and so on.

Keywords: Discrete Particle Simulation, Sense Phase Flow, Multi-Scale Analysis, DEM, DSMC

1. INTRODUCTION

In general, research of natural phenomena is made on various levels of scale, from micro to macro scale. Meso-scale approach lies between micro-scale and macro-scale ones. The boundaries between these scales depend on research subjects and view points of researchers. In some cases, the micro-scale approach corresponds to the molecular level and in other cases, the micro-scale is not necessarily as small as the size of molecules. Historically, research in engineering has been developing in the order of macro, meso and micro scales. Each of micro, meso and macro scale approaches has its own values and roles. When dealing with industrial phenomena in large facilities, the macro-scale approach is usually inevitable in practice. In such macro-scale approaches, various empirical factors have been used in the formulation. In the framework of multi-scale formulation, such factors in the macro-scale approach are expected to be determined by meso-scale approach. The meso-scale approach also includes empirical factors. Such empirical factors in the meso-scale are expected to be determined by the micro-scale one. Therefore, approach of each scale is linked with the other. If you are a scientist, your final goal might be to understand the phenomena in the micro scale which is regarded as the most basic way. When considering engineering applications of our research, you must provide tools to engineers which should be convenient to predict macro-scale properties. Thus if you are engineering-oriented scientist, you must ply between the micro-scale and the macro scale via the meso-scale viewpoint. In this paper, numerical analysis of gas-particle flows is classified based the above view point.

2. CLASSIFICATION

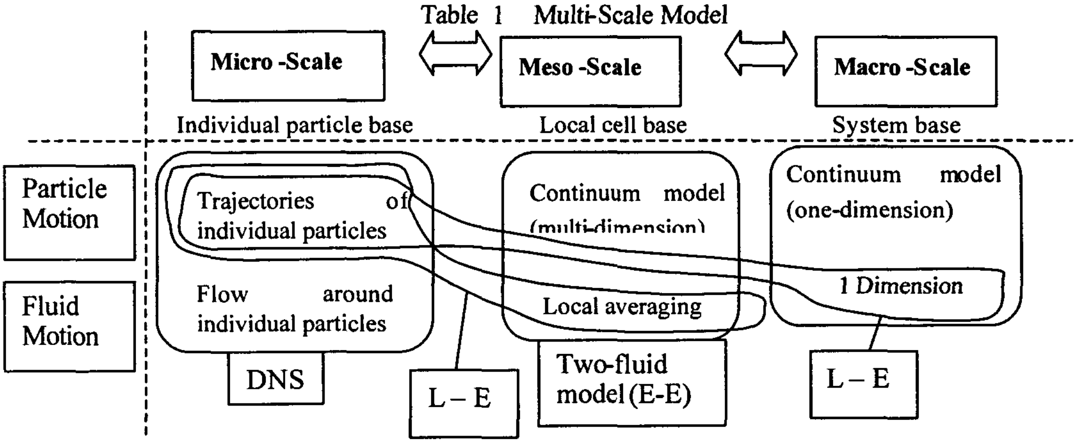
Methods of numerical analysis of particle-fluid flows is arranged and classified using the concept of scales; micro-, meso- and macro-scale as shown in Table 1.The micro-scale method corresponds to individual particle base, the meso-scale method to local cell base and the macro-scale method corresponds to system base. In the micro-scale method of particle motion, trajectories of individual particles are calculated by using the equations of particle motion. The meso-scale method is called the continuum model because an assemblage of particles is regarded as a fluid. In the macro-scale method, an assemblage of particles is assumed to be a fluid as well but the mathematical treatment is one-dimensional. The fluid phase is analyzed in the same concept as the particle phase; that is, in the micro-scale method, flow around individual particles is calculated, and in the meso-scale analysis of fluid motion, flow around particles is not calculated, but fluid motion corresponding to the calculation cell in which several particles exist is calculated. The effects of particles on fluid is averaged within the cell. In the macro-scale analysis of fluid motion, fluid motion is treated one-dimensionally in the same way as in the case of particle motion. The mean velocity averaged in the cross section is handled. The pressure drop is a typical quantity in the macro-scale method.

Analytical methods of multiphase flows which have been developed up to the present are classified into the following 5 cases.

Case 1 : Particle – macro, Fluid – macro
Case 2 : Particle – meso, Fluid – meso
Case 3 : Particle – micro, Fluid – micro
Case 4 : Particle – micro, Fluid - macro
Case 5 : Particle – micro, Fluid - meso

Case 1 (Particle – macro, Fluid – macro) is most industry-oriented and it is easy to use. Case 2 (Particle – meso, Fluid – meso) is called two-fluid model or Eulerian- Eulerian method. This method is popular among many commercial soft wares. Case 3 (Particle – micro, Fluid – micro) is called DNS (Direct Numerical Simulation). This method is most rigorous but much time and large memories are needed to get results. Case 4 and Case 5 are called Lagrangian-Lagrangian method.

Table 1 Multi-Scale Model



Next, the micro-scale method of particle motion is explained.

2.1 Micro-scale approach of particle motion

In the micro-scale approach, trajectories of individual particles are calculated by using the equations of particle motion.. From the view point of particle-particle interaction, this approach is classified into the following three cases.

Collision free flow

Collision dominated flow

Contact dominated flow

The collision free flow corresponds to dilute phase flows and thus it is not discussed in this paper dealing with dense phase flows. The collision free flow corresponds to dilute phase flows. The collision dominated flow corresponds to dispersed flow but not so dilute. The contact dominated flow corresponds to dense phase flows. The presence of fluid is pre-requisite in the collision free and collision dominated flows. In the contact dominated flow, the presence of fluid is not necessarily considered. Thus, applications of contact dominated flow is divided into the cases with and without fluid effects.

2.1.1 Collision dominated flows

Particles change their velocities due to collision. This change in velocities can be calculated by the so-called hard particle model. The relation between the pre- and post-collision velocities is given explicitly using the coefficient of restitution and friction coefficient [1,2]. When the particulate phase is dispersed in gas, it is sufficient to consider only simple binary collision and not multiple collision. The difficulty associated with collision is how to find collision pairs from a large number of particles. There are two methods available for this problem. The one is to find pairs deterministically from trajectories of individual particles[3]. As the particle number increases, long CPU time and large memories are needed in this method. Another method is based on the probability of collision [3-5]. DSMC(Direct Simulation Monte Carlo) method is known as such a method. In the DSMC method, calculation is made for only sample particles. There is no limit of particle number in the system.

2.1.2 Contact dominated flow

Before considering the model for contact dominated flows, let us consider a particle is approaching other particles and contacts or collides as shown

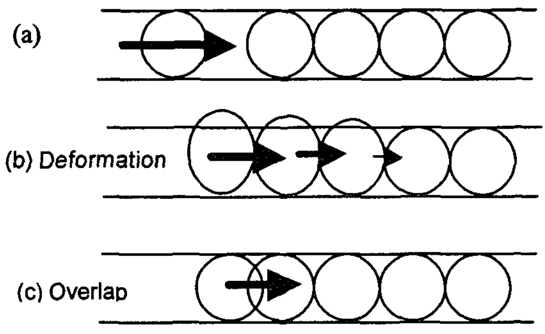
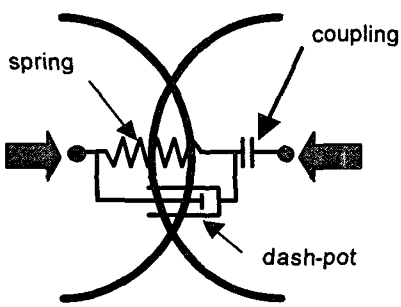


Fig. 1 Particle-particle contact (collision)

in Fig. 1a If this phenomenon is described very precisely, it is found that all particles deform, larger or smaller. The deformation is transmitted and decayed, as shown in Fig. 1b. As is easily imagined, it is difficult in practical calculations to calculate change of shape which is a function of force acting on the particle. Thus, instead of considering the deformation, the particles are made overlap as shown in Fig. 1c. The overlap distance corresponds to the rate of deformation. The more the overlap distance, the larger the repulsive force. Further it is assumed that the influence of the particle of interest is limited to only neighboring particles which contact that particle in direct.

Once the above assumption is adopted, modeling is relatively easy. The so called soft particle model is used to estimate the effects of contact on particle motion. The soft particle model is usually modeled by using a spring, dash pot and slider as shown in Fig. 2 [10]. In general, several particles are in contact with a particle at the same time. Therefore the total force and torque acting on the particle is obtained by taking the sum of forces due to surrounding particles contacting it.



(a) normal force

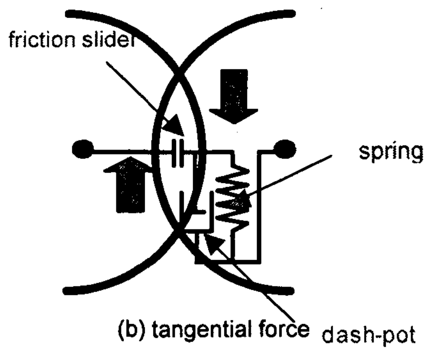


Fig.2 Model of contact force

The method using the model shown in Fig. 1 is called "Discrete Element Method", "Distinct Element Method" or shortly "DEM". This model has been used to calculate soil or rock flows. Typical examples of contact dominated flows in multiphase flows are dense phase pneumatic conveying and fluidized bed. Tsuji et al. [11] took into account the effect of gas in DEM and began with dense phase pneumatic conveying. Tsuji et al. [12] extended their work to fluidized bed as shown later.

2.2 Meso-scale approach of particle motion

An assemblage of particles is regarded as a fluid in the meso-scale approach. The most earliest model categorized into this group is the one made by Davidson[13]. He analyzed the bubble motion in fluidized beds using the potential flow theory. His theory and others following the same approaches are described in detail in the monograph written by R. Jackson[14].

If the mixture is assumed to be made of real gas and particle fluid, this model is called two-fluid model. The two fluid model is currently most popular in the field of multiphase flow calculations. Since an assemblage of particles is treated as a fluid, it is necessary to specify its density and viscosity. Several correlation terms of fluctuating velocities similar to the Reynolds stresses in single phase flow should also be specified in turbulent two-phase flows. Particles have various properties, such as geometric properties (mean size, size distribution, shape) , cohesion properties and thermal properties. The phenomena of multiphase flows are affected by these properties. In the continuum models, these properties should be given by mathematical expressions. However, it is difficult to deduce the expressions which have wide ranges of applications. It is relatively easy for the micro-scale approach to take into account these properties. For instance, the cohesion force caused by liquid bridges can be taken into account in the micro-scale approach [15,16].

In general, the micro-scale approach is not suitable for large scale phenomena. Nevertheless it is expected that the micro-scale approach is helpful in deducing reasonable mathematical expressions of particle properties for meso-scale approach. The kinetic theory can be regarded as such an approach. In the kinetic theory, the constitutive equations in the continuum model are deduced from equations of particle motion in the same way as the constitutive equations in Navier-Stokes equation are deduced from the Boltzman equation. The reference [17] is informative concerning the kinetic theory. The kinetic theory is being improved and is called PDF approach recently. The recent state of PDF approach can be seen in the paper by Reeks [18]

2.3 Macro-scale approach of particle and fluid motion

The macro-scale approach of particle and fluid motion can be defined as the one which does not deal with two or three dimensional quantities but over all quantities. If the velocity field is the matter, velocity averaged over cross section and flow rates are main concerns. If the pressure field is the matter, pressure drop or pressure gradient is investigated.

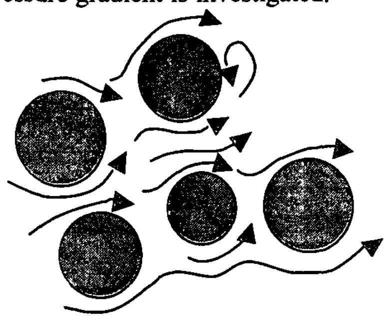


Fig. 3 Micro-scale approach of fluid motion

2.4 Micro-scale approach of fluid motion

The micro-scale approach of fluid motion is rapidly developing in the last 10 years. This approach is applied in the main to liquid-particle flows. In the micro-scale approach, the flow around each particle is solved based on the full Navier-Stokes equation [19-23] as shown in Fig. 3. The Lattice-Boltzmann simulation [24] also has been applied to fluidization. The fluid forces acting on particles are estimated by integrating stresses on the surface of particles which are solutions of the basic equation. Thus, empirical coefficients associated with drag and lift forces are not necessary in the micro-scale approach. Drag and lift coefficients described in text books and monographs are valid when the particle is fixed in the space where the fluid moves at the relative velocity of fluid and particle. Actually the instantaneous motion of a flying particle is affected by the flow which the particle itself produces. A typical example of this case is the particle motion affected by the vortex behind the particle.

2.5 Meso-scale approach of fluid motion

In the meso-scale treatment a flow field is divided into cells (Fig. 4),, the size of which should be larger than the particle size and smaller than the macro-scopic size of the flow field like a pipe diameter. The effects of the presence of particles on the fluid are taken into account by void fraction of each phase and momentum exchange through drag force. This approach can be called "local averaging approach". The meso-scale treatment developed by Anderson and Jackson [25] is quite common in numerical analysis of multiphase flows, although the word "meso-scale" was not used when Anderson and Jackson [25] developed their model.

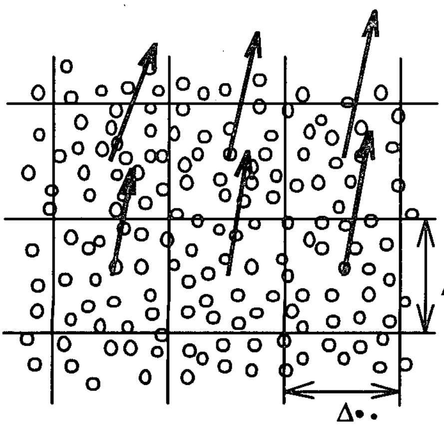


Fig.4 Meso-scale approach of fluid motion

EXAMPLES

Examples of numerical simulation of dense phase particle-gas flows are shown for the the following cases.

Case 2 : Particle – meso, Fluid – meso
Case 3 : Particle – micro, Fluid – micro
Case 4 : Particle – micro, Fluid - macro
Case 5 : Particle – micro, Fluid - meso

Case 2 (Particle – meso, Fluid – meso)

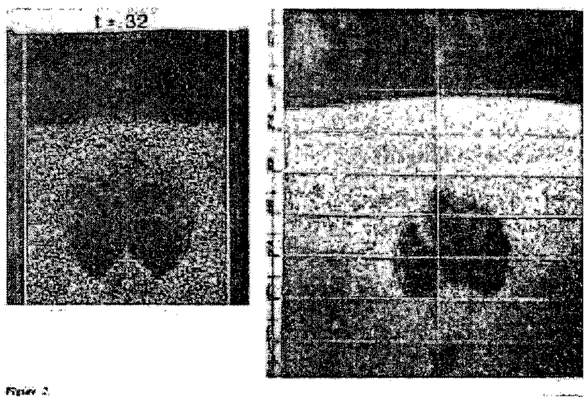
The Gidaspow's group (Illinois Institute of Technology) is a representative of the meso-scale approach for particle and fluid. Fig. 5 shows the result of Gidaspow's work.

Case 4 :(Particle – micro, Fluid – macro)

Typical examples of contact dominated flows in multiphase flows are dense phase pneumatic conveying and fluidized bed. Tsuji et al. [11] took into account the effect of gas in DEM and began with dense phase pneumatic conveying. Fig. 6 shows the result.

Case 3 : Partcie – micro, Fluid – meso

This approach is preferred by the Tsuji and Tanaka group (Osaka University). They showed several eaxmples where particle-particle interaction plays important roles. Fig. 7 shows a snap shop of particle concentration and velocity vectors of particles and gas calculated by the



Calculation Experiment

Fig. 5 Two-dimensional fluidized bed calculated by Gidaspow and Seo [26]

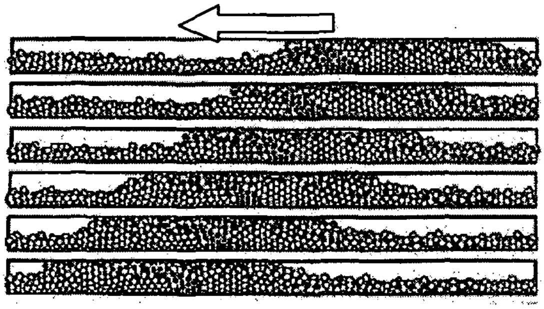


Fig. 6 Plug conveying in horizontal pipe [11]

DSMC method [5]. The interesting finding is that the in-elastic particle-particle collision leads to the formation of clusters. Corresponding to the clusters, the flow field shows large scale fluctuation.

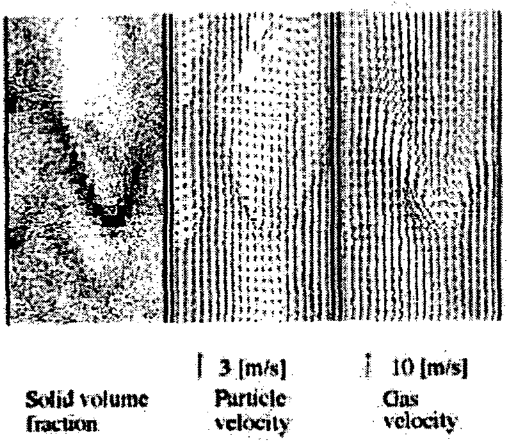


Fig. 7. Flow around a cluster [5]

Fig. 8 shows a single rising bubble in two-dimensional fluidized bed calculated by DEM. Fig.9 shows calculated result of three-dimensional spoted bed.[12]

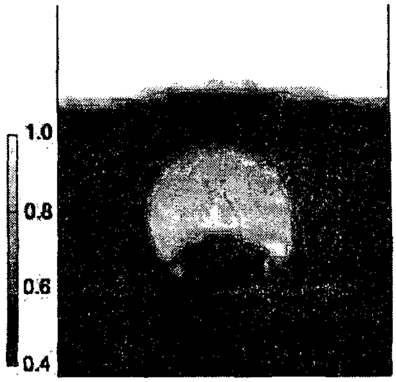


Fig. 8 Single rising bubble in fluidized bed
Particle number =290,000,
Particle Size = 1.3 mm

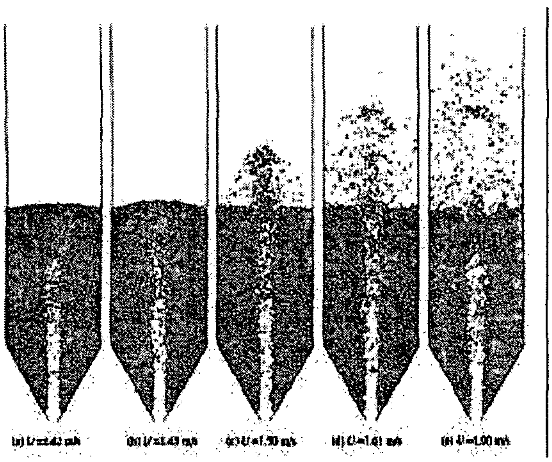


Fig. 9 Spouted bed

Fig. 10 Snap shot of falling particles in the fluid [22]

Case 4 : Particle – micro, Gas - micro

Dan Joseph group I(University of Minnesota) is well known for the micro-scale approach for particle and fluid this approach [23]. Another researcher active in this kind of
calculation is Kajishima [22]. Fig.10 shows particles falling in the fluid under the effect of gravity. Shedding vortices
are calculated for each particle.

The author calls the particle micro approach "discrete particle simulation." . The author and his group have made many simulations of partiuculate flows. They classify examples into the following three cases based on particle-particle interaction.

1. Collision free flow
2. Collision dominated flow
3. Contact dominated flow

Examples of are presented in Table 2. There are so many papers reported up to the present that presenting references of individual works are omitted in this paper. In stead, references [27-29] are cited here for showing the recent trend of research and applications. In the preceding sections, a few monographs [1, 14, 17] are cited for references. Two more monographs [30,31] are added here as references relevant to the present topic.

Table 2 Examples of applications of discrete particle simulation
(The asterisk * means the examples which the author's laboratory experienced.)

(1) Collision free flow		Turbulent diffusion, Dust collection, Dilute phase transport of particles* (pneumatic or hydraulic)
(2) Collision dominated flow		*Circulating fluidized bed**, Particle transport at intermediate concentration* (pneumatic or hydraulic)
(3) Contact dominated flow	Effect of fluid : Neglected	Soil flow, Avalanche, Compaction, Simple shear flow*, Vibrating bed*, Hopper* & chute flow, Ball mill*, Rotating drum*, Screw feeder*, Mixer*, Granulator*, Shock absorber*, Crush*, Sieve, Copy machine*
	Effect of fluid: Considered	Fluidized bed*, Dense phase transport*, Colloid*

REFERENCES

1. Crowe, C., Sommerfeld, M., Tsuji, Y., 1997, "Multiphase Flows with Droplets and Particles," CRC Press, pp.128-133.
2. Tanaka, T., Tsuji, Y., 1991, "Numerical simulation of gas-solid two-phase flow in a vertical pipe: On the effect of inter-particle collision," Gas-Solid Flows ASME FED-vol.121, Stock et al. eds, pp.123-128
3. Sommerfeld, M and Zivkovic, G., 1992, "Recent advances in the numerical simulation of pneumatic conveying through pipe systems," Computational Method in Applied Science First Europian Computational Fluid Dynamics, Hirsch, et al. eds, pp.201-212.
4. Oesterle, B. and Petitjean, A., 1993, "Simulation of particle-to-particle interactions in gas-solid flows, Int. Journal of Multiphase Flow 19, pp.199-211.
5. Yonemura, S., Tanaka, T. and Tsuji, Y., 1993. Cluster Formation in Gas-Solid Flow Predicted by DSMC Method, ASME/FED Gas-Solid Flows Vol.166, 303-309.
6. Crowe, C., Sommerfeld, M., Tsuji, T., 1997, "Multiphase Flows with Droplets and Particles," CRC Press, pp.20-22.
7. Yamamoto, Y., Potthoff, M., Tanaka, T., Kajishima, T., and Tsuji., Y., *2001*, "Large-eddy simulation of turbulent gas-particle flow in a vertical channel: effect of considering inter-particle collisions," Journal of Fluid Mechanics, Vol.442, pp. 303-334.
8. Berlemont, A., Achim, P. and Chang, Z., 2001, "Lagrangian approaches for particle collisions: The colliding particle velocity correlation in the multiple particle tracking method and in the stochastic approach," Phys. Fluids 11-10, pp. 2926-2956
9. Sakiz, M. and Simonin, O., 2001, "Continuum modeling and Lagrangian simulation of massive frictional colliding particles in a vertical gas-solid channel flow," 4th Int. Conf. On Multiphase Flow, ICMF'01, New Orleans, USA, May 27 June Paper No. 186 (CD-ROM)
10. Cundall, P. A. and O. D. Strack, O. D., 1979, "A discrete numerical model for granular assemblies", . Geotechnique 29-1, 47.
11. Tsuji, Y., Tanaka, T., Ishida, T., 1992. Lagrangian Numerical Simulation of Plug Flow of Cohesionless Particles in a Horizontal Pipe. Powder Technology 71, 239-250
12. Tsuji, Y., Kawaguchi, T. and Tanaka, T., 1993. Discrete Particle Simulation of Two-Dimensional fluidized Bed, Powder Technology 77, 79-87.
13. J. F. Davidson, J. F., 1961, "Symposium on fluidization-discussion," Trans. Inst. Chem. Eng. 39, pp.230-232
14. Jackson, R., 2000, "The Dynamics of Fluidized Particles, " Cambridge University Press, pp.157-176
15. Thornton, C., Lian, G. and Adams,M. J., 1993, "Modelling of liquid bridges between particles in DEM simulations of particle systems," Proceedings, 2nd International Conference on Discrete Element Methods (DEM), J. R. Williams and G. G. W. Mustoe, eds., IESL Publications, Cambridge, MA, USA, pp.177-187.
16. Muguruma, Y., Tanaka, T. and Tsuji, Y., 2000, "Numerical simulation of particulate flow with liquid bridge between particles simulation of centrifugal tumbling granulator," Powder Technology, Vol. 109, pp. 49-57.
17. Gidaspow, D., 1997, "Multiphase Flow and Fluidization, pp.239-296.
18. Reeks ,M., 2003, "Comparison of Recent Model *Equations for Particle Dispersion in a Turbulent* Boundary Layer with Those Based on the PDF Approach," ASME/FED Gas-Particle Flows, FEDSM2003-45734
19. Hu, H. H., 1996. Direct simulation of flows of solid-liquid mixtures. Int. J.Multiphase Flow, 22 (2), 335-352.
20. Pan, Y. and Banerjee, S., 1996, "Numerical simulation of particle interactions with wall turbulence," Phys. Fluids, 8:2733-2755,
21. Pan, Y. and Banerjee, S., 1997, "Numerical investigation of the effect of large particle on wakk turbulence," Phys. Fluids 9: 3786-3807
22. Kajishima,T. and Takiguchi, S., 2002, "Interaction between particle clusters an particle-induced turbulence," Int. J. Heat and Fluid Flow 23, pp.639-646
23. Pan, T. W. , Joseph, D. D., Bai, R., Glowinski, R. and Sarin, V. J., 2002 , "*Fluidization of 1204* spheres: simulation and experiment, J. Fluid Mech., 451, p.169,.

24. Qi, D., 2000, "Lattice-Boltzmann simulations of fluidization of rectangular particles," Journal of Multiphase Flow 26, pp.421-433.
25. Anderson, T. B. and Jackson, R., 1967, A Fluid Mechanical Description of Fluidized Beds. I & EC Fundamentals 6, 527.
26. Gidaspow, D. and Seo, Y. C., 1986, "Hydrodynamics of Fluidization: Supercomputer generated vs. experimental bubbles," J. of Powder & Bulk Solkids Technology 10-3, pp. 19-23..
27. Powder technology, Vol.109, Issues 1-3 2000, pp.1-298, Numerical Simulations of Discrete Particle Systems
28. Proc. of the Third International Conference on Discrete Element Methods, (Santa Fe, New Mixico, US, 2002)
29. Tsuji, Y., 2000, "Activities in discrete particle simulation in Japan, " Powder Technology 113, 278-286
30. Zhou, L, 2000, "Theory and Numerical Modeling of Turbulent Gas-Particle Flows and Combustion, CRC Press
31. Fan, L-S. and Zhu, C., 1998, "Principles of Gas-Solid Flows," Cambridge University Press