

EFFECT OF MODEL FORMULATION OF DISCRETE PARTICLE SIMULATION ON THE GAS FLUIDIZATION BEHAVIOUR

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ABSTRACT

Discrete particle simulation has been recognised as a useful numerical technique to elucidate the fundamentals governing gas-solid flow in fluidisation. In general, it is achieved by combining the discrete flow of a particle phase with the continuum flow of a gas phase; however, different model formulations have been used in the literature, and their effect is not fully understood. This paper attempts to address this matter. The governing equations used are related to the so-called Model A and Model B which give different interpretations of particle-fluid interaction in the well-established two fluid model. Their difference is quantified by a numerical simulation of two cases: fluidization of mono- or bi-sized particles. Physical experiments are conducted to help clarify this matter.

NOMENCLATURE

$C_{d0,i}$	drag coefficient on an isolated particle i , dimensionless
E	Young's modulus, Nm^{-2}
$\mathbf{f}$	contact, drag or gravitational force, N
$\mathbf{F}$	volumetric fluid-particle interaction force, Nm^{-3}
g	gravitational acceleration, ms^{-2}
I	rotational inertia momentum of particle, kgm^2
k_c	number of particles in a computational cell, dimensionless
k_i	number of particles in contact with i , dimensionless
m	mass, kg
P	pressure, Pa
R_i	particle radius, m
$\mathbf{R}_i$	vector of magnitude R_i from the mass centre of particle i to a contact point, m
$\text{Re}_{p,i}$	Reynolds number of particle i , dimensionless
t	time, s
T	torque, Nm
$\mathbf{u}$	gas velocity, ms^{-1}
$\mathbf{v}$	solid velocity, ms^{-1}
V	volume, m^3
ΔV	volume of computational cell, m^3
$\delta_{t,ij}$	vector of the accumulated tangential displacement between particles i and j , m
$\mathcal{E}$	porosity, dimensionless
μ	viscosity, $\text{kgm}^{-1}\text{s}^{-1}$
η_n	normal and tangential damping coefficients, dimensionless
η_t	normal and tangential damping coefficients, dimensionless
ρ	density, kg/m^3
ω	rotational velocity of particle, s^{-1}

$\boldsymbol{\tau}$	viscous stress tensor of gas, $\text{kgm}^{-1}\text{s}^{-2}$
ν	Poisson ratio, Nm^{-1}

SUBSCRIPTS

c	contact
d	damping
f	fluid phase
i	particle i
j	particle j
p	particle

INTRODUCTION

Gas-solid flow can be found both in nature and in various industrial processes and has been a subject of intensive research, particularly for gas fluidisation (Geldart, 1973; Davidson et al, 1985). Physical modelling has been widely used to understand fluidization phenomena in the past. However, a comprehensive understanding of the flow system is still difficult due to the limitation of measurement techniques, particularly in relation to the micro-dynamics at a particle scale, such as the trajectories of and forces acting on individual particles which are believed to be key to elucidating the governing mechanisms. Numerical modelling is an effective approach to obtain such particle scale information, mainly achieved by a recently developed Combined Continuum and Discrete Model (CCDM). The key feature of CCDM is solving particle flow by use of the Discrete Element Method (DEM) and gas flow by Computation Fluid Dynamics (CFD) with their coupling through the particle fluid interaction force. This model can generate detailed information about solid phase (such as trajectories of particles, particle-particle and particle-fluid interaction forces) in comparison with the Two Fluid Model (TFM) (Gidaspow, 1994). This technique attracts more and more attention worldwide as briefly reviewed by Yu and Xu (2003). However, differences exist in implementing this technique in actual numerical simulations, mainly reflected on the governing equations in relation to the so-called Model A, which treats the pressure drop in both the solid and gas phases, and Model B, which treats the pressure drop in the gas phase only. Differences also occur for the schemes for coupling gas and solid phases which are modelled at different length scales, and on the equations for quantifying the particle-fluid interaction forces.

A comparison of the effect of different model formulations has been conducted both in TFM (Bouillard et al, 1989) and in CCDM (Kafui et al, 2002). The TFM comparison shows no major difference although Model B is considered to be well-posed while Model A ill-posed. The CCDM comparison also shows a minor difference in qualitative fluidisation phenomena, but a significant

difference in the bed expansion in the first wave of bed expansion and in the comparison of simulated pressure drop-superficial gas velocity with empirical correlations in the fixed bed regime. However, the results of Kafui et al (2002) deserve further discussion, as different initial packing conditions were used, also an acceleration term is added to their Pressure Gradient Force (PGF) model (in essence Model A), but not to their Fluid Density-Based Buoyancy (FDB) model (in essence Model B).

This paper presents our study on this topic. Simulations are conducted not only on mono-sized systems with the same condition as the one used by Kafui et al (2002), but also on a bi-sized system. Experiments are conducted under comparable conditions to help clarify this matter.

MODEL DESCRIPTION

In CCDM, the gas phase is treated by a continuum approach, and its flow complies with the law of conservation of mass or momentum. The governing equations are the same as those used in the well-established TFM (see, for example, Gidaspow, 1994). Two formulations have been proposed depending on the method to treat pressure drop, referred to as model A and model B. Both models have been used in CCDM (for example, see Tsuji et al. (1993) for Model A and Xu and Yu (1997) for Model B), their corresponding governing equations for gas phase can be expressed as

Conservation of mass:

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \mathbf{u}) = 0 \quad (1)$$

Conservation of momentum:

Model A:

$$\frac{\partial \rho_g \varepsilon_g \mathbf{u}_g}{\partial t} + \nabla \cdot (\rho_g \varepsilon_g \mathbf{u}_g \mathbf{u}_g) = -\varepsilon_g \nabla P - \mathbf{F}^A + \varepsilon_g \nabla \tau_g + \rho_g \varepsilon_g \mathbf{g} \quad (2a)$$

Model B:

$$\frac{\partial \rho_g \varepsilon_g \mathbf{u}_g}{\partial t} + \nabla \cdot (\rho_g \varepsilon_g \mathbf{u}_g \mathbf{u}_g) = -\nabla P - \mathbf{F}^B + \varepsilon_g \nabla \tau_g + \rho_g \varepsilon_g \mathbf{g} \quad (2b)$$

where $\mathbf{u}$ and P are, respectively, the fluid velocity and pressure; τ , ε , ρ_g and ΔV are the fluid viscous stress tensor, porosity, density and volume of a computational cell, $\mathbf{F}^A$ and $\mathbf{F}^B$ are the volumetric particle-fluid interaction forces for models A and B respectively.

The solid phase is treated by a discrete approach. Two types of motion of individual particles (translation and rotation) are directly determined by Newton's second law of motion. The forces acting on individual particle include gravitational force, contact forces between particle and particle, particle and wall, and interaction forces between particle and fluid. Therefore, the governing equations for particle i can be expressed as

$$m_{p,i} \frac{d\mathbf{u}_{p,i}}{dt} = \mathbf{f}_{p-f,i} + \sum_{j=1}^{k_i} (\mathbf{f}_{c,ij} + \mathbf{f}_{d,ij}) + \rho_{p,i} V_{p,i} \mathbf{g} \quad (3)$$

for translational motion and

$$I_i \frac{d\omega_i}{dt} = \sum_{j=1}^{k_i} \mathbf{T}_{ij} \quad (4)$$

for rotational motion. Here m_i , I_i , k_i , $\mathbf{u}_{p,i}$ and ω_i are, respectively, the mass, moment of inertia, number of contacting particles, translational and rotational velocities of particle i ; $\mathbf{f}_{c,ij}$, $\mathbf{f}_{d,ij}$ and $\mathbf{T}_{ij}$ are the contact force, viscous contact damping force and torque between particles i and j . These inter-particle forces and torques are summed over the k_i particles in contact with particle i . $\mathbf{f}_{p-f,i}$ is the particle

fluid interaction force, which includes many forms, such as fluid drag force ($\mathbf{f}_{d,i}$), buoyancy force, lifting force, etc. Here only buoyancy and fluid drag force are considered. The particle fluid interaction force is calculated in two formulations corresponding to Eq. (2) for gas phase. That is

Model A:

$$\mathbf{f}_{p-f,i} = -V_{p,i} \nabla P_i + \mathbf{f}_{p-f,i}^A \quad (5a)$$

Model B:

$$\mathbf{f}_{p-f,i} = \rho_g V_{p,i} \mathbf{g} + \mathbf{f}_{p-f,i}^B \quad (5b)$$

The particle fluid interaction force is formed by two terms in both equations. The first part is the buoyancy part which is related to the local pressure drop for Model A while only the static pressure drop for Model B. The second part is related to fluid drag force ($\mathbf{f}_{drag,i}$). As noted by Xu and Yu (1998), for gas fluidisation, in Model B, the second term are exactly the fluid drag force ($\mathbf{f}_{drag,i}$), while in Model A, it has the relationship with drag force ($\mathbf{f}_{p-f,i} = \varepsilon_g \mathbf{f}_{drag,i}$). Consistency in equation formulation is important to avoid unreal results.

The formulations used to calculate the forces and torques involved in Eqs (3) and (4) are listed in Table 1. Note that the fluid drag force is calculated according to Di Felice's correlation (1994), which can eliminate the discontinuity resulting from Ergun equation (1952) and Wen & Yu's correlation (1956) at porosity 0.8 as shown in Figure 1 where the gas density and viscosity used is 1.205 kgm^{-3} and $1.8 \times 10^{-5} \text{ kgm}^{-1}\text{s}^{-1}$ respectively. Which equation is more accurate probably deserves further study, but is beyond the scope of this work.

Coupling between the gas and solid phases at each time step is achieved by calculating the particle fluid interaction force for individual particles which is then used for the gas phase through local averaged scheme as given by Eq. (6).

$$\mathbf{F} = \frac{\sum_{i=1}^{k_c} \mathbf{f}_{g-p,i}}{\Delta V} \quad (6)$$

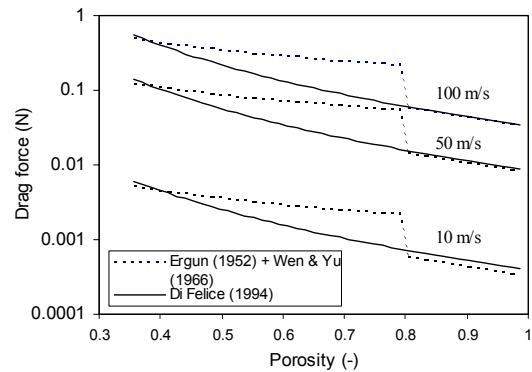


Figure 1 Drag forces acting on a 4 mm diameter particle as a function of porosity for different apparent gas velocities.

RESULTS AND DISCUSSION

To identify the effect of model formulations, numerical simulations are conducted for mono- and bi-sized fluidization systems.

Mono-sized system

For the mono-sized system, simulations are conducted in a pseudo-2D bed with the bed thickness identical to the

particle diameter. The parameters are listed in Table 2, actually similar to those used in Kafui et al's simulation. Initial packing is obtained by randomly generating particles without overlap in the whole bed, and allowing

them to fall down under gravity for 1 second. To make the simulation results comparable, the same initial packing is used in the assessment of two model formulations. Gas is injected from the bottom uniformly at velocity 2.5 m/s.

Forces and torque		Symbols	Equations
Normal forces	Contact	$\mathbf{f}_{cn,ij}$	$-\frac{4}{3}E^*\sqrt{R^*\delta_n^{\frac{3}{2}}}\mathbf{n}$
	Damping	$\mathbf{f}_{dn,ij}$	$-\eta_n\left(6m_{ij}E^*\sqrt{R^*\delta_n}\right)^{\frac{1}{2}}\mathbf{v}_{n,ij}$
Tangential forces	Contact	$\mathbf{f}_{ct,ij}$	$-\frac{\mu_s\mathbf{f}_{cn,ij}}{ \delta_{t,ij} }\left[1-\left(1-\frac{\min\{\delta_{t,ij},\delta_{t,ij,max}\}}{\delta_{t,ij,max}}\right)\right]\delta_{t,ij}$
	Damping	$\mathbf{f}_{dt,ij}$	$-\eta_t\left(6m_{ij}\mu_sF_{cn,ij}\frac{\sqrt{1-\delta_{t,ij}/\delta_{t,ij,max}}}{\delta_{t,ij,max}}\right)\delta_{t,ij}\mathbf{v}_{t,ij}$
Fluid drag force		$\mathbf{f}_{fi}$	$0.5c_{d0,i}\rho_f\pi R_i^2 \mathbf{u}_i-\mathbf{v}_i (\mathbf{u}_i-\mathbf{v}_i)\epsilon_i^{1-\chi}$
Torque		$\mathbf{T}_{ij}$	$\mathbf{R}_i\times(\mathbf{F}_{ct,ij}+\mathbf{F}_{dt,ij})$
Gravity		$\mathbf{f}_{gi}$	$m_i\mathbf{g}$
where: $\frac{1}{R^*}=\frac{1}{R_i}+\frac{1}{R_j}$, $E^*=\frac{E}{2(1-\nu^2)}$, $\mathbf{n}=\frac{\mathbf{R}_i}{R_i}$, $\delta_{t,ij,max}=\mu_s\frac{2-\nu}{2(1-\nu)}\delta_n$, $m_{ij}=\frac{m_i+m_j}{2}$, $\mathbf{v}_{ij}=\mathbf{v}_j-\mathbf{v}_i+\boldsymbol{\omega}_j\times\mathbf{R}_j-\boldsymbol{\omega}_i\times\mathbf{R}_i$, $\mathbf{v}_{n,ij}=(\mathbf{v}_{ij}\bullet\mathbf{n})\bullet\mathbf{n}$, $\mathbf{v}_{t,ij}=(\mathbf{v}_{ij}\times\mathbf{n})\times\mathbf{n}$, $c_{d0,i}=\left(0.63+\frac{4.8}{\text{Re}_{p,i}^{0.5}}\right)^2$, $\text{Re}_{p,i}=\frac{2\rho_f R_i \epsilon_i \mathbf{u}_i-\mathbf{v}_i }{\mu_f}$, $\chi=3.7-0.65\exp\left[-\frac{(1.5-\log_{10}\text{Re}_{p,i})^2}{2}\right]$			

Table 1 Components of forces and torque acting on particle i from particle j.

Solid phase	
Number of particles	2,400
Density (kgm ⁻³)	2,700
Young's Module (Nm ⁻²)	6.895×10 ¹⁰
Poisson ratio (Nm ⁻¹)	0.33
Friction coefficient (-)	0.33
Damping coefficient (-)	0.3
Diameter (m)	0.004
Gas phase	
Viscosity (kgm ⁻¹ s ⁻¹)	1.8×10 ⁻⁵
Density (kg/m ³)	1.205
Bed height (m)	0.9
Bed width (m)	0.15
Bed thickness (m)	0.004
Cell width (m)	0.010
Cell height (m)	0.010

Table 2 Parameters used for mono-sized systems

Comparison was firstly checked on the initial response of the bed to the introduction of the gas (2.5 m/s) as shown in Figure 2. Typical slugging phenomena corresponding to a Geldard group D behaviour can be seen in both model formulations. Both of their maximum bed height for the first wave of particle flow happen around 0.4 s, and has a value of 0.38 m which is about 150% of the initial bed height. The subsequent flow patterns are also given here as shown in Figure 3 which shows a minor difference. This is also the case when checking the variation of maximum bed height (Figure 4) and pressure drop (Figure 5). Therefore, for mono-sized systems, Model A and Model B produce comparable results, and the minor

difference is probably difficult to be experimentally identified. This remark is consistent with the TFM approach (Bouillard et al, 1989).

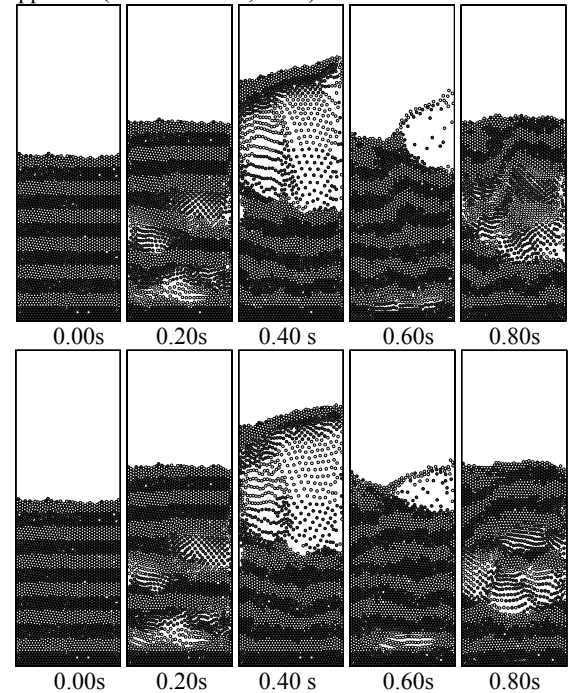


Figure 2 The initial response of the bed to the introduction of gas injection at a velocity of 2.5 m/s: Model A (top); Model B (bottom).

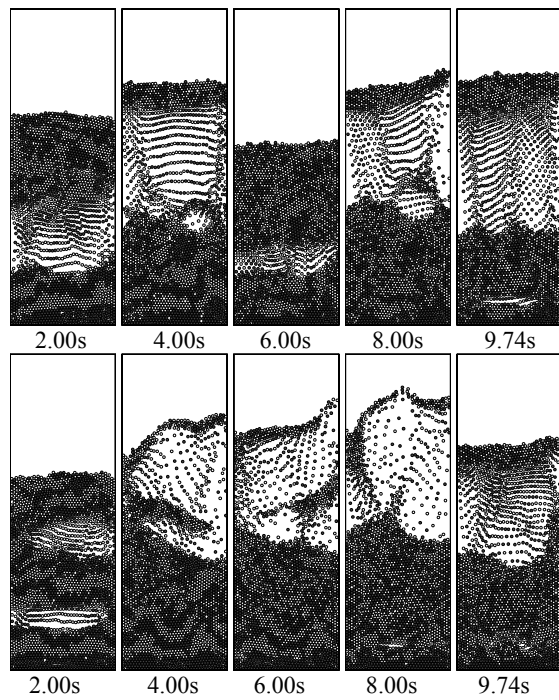


Figure 3 Typical flow patterns at velocity 2.5 m/s: Model A (top); Model B (bottom).

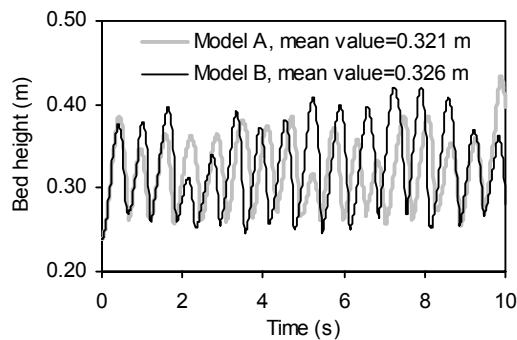


Figure 4 Variation of maximum bed height with time

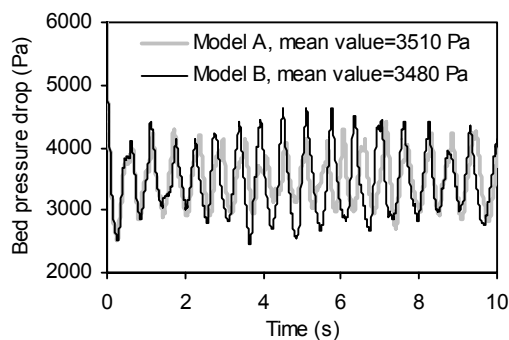


Figure 5 Variation of pressure drop with time

These results generally agree with the previous simulation (Kafui et al, 2002), except for the initial response of the bed to the introduction of gas injection. Our simulation shows little difference in the bed expansion, while in Kafui et al's simulation, the maximum bed height for the first wave of particle flow is 120% higher than the initial bed height with Model A and 30% with Model B. There are a few reasons responsible for this difference. First, Kafui et al. (2002) actually used two different initial packed beds for their fluidisation simulation. The beds

were produced from de-fluidisation at two different gas velocities: 2.5 m/s for Model A, and 3.0 m/s for Model B. Consequently, the bed porosity differs: 0.446 for Model A and 0.464 for Model B. It is well known that the pressure drop or fluid drag force is very sensitive to porosity, especially in dense packing regions as seen in Figure 1. To be specific, the pressure drops as a function of superficial velocities for the two beds are plotted in Figure 6. The total bed weight (3545 Pa) is also plotted for convenience. Clearly, the denser packing corresponds to a larger value of pressure drop at a given superficial velocity. When the gas injection velocity is 2.5 m/s, we obtain that the pressure drop is 5065 Pa for porosity 0.446 and 4250 Pa for porosity 0.464, calculated analytically by Di Felice's equation. Subtracting the static bed pressure (3545 Pa), we can obtain an extra pressure drop contributing to the bed expansion of 1520 Pa for porosity 0.446 and 705 Pa for porosity 0.464. These are equivalent to 43% and 20% of the bed weight respectively. It is doubtless that this will cause a larger bed expansion for porosity 0.446 than porosity 0.464.

Another deficiency in the approach of Kafui et al. is that the viscous stress tensor term is added to their Model A simulation, but not to their Model B simulation. This term is often ignored in gas fluidisation because of the significant difference in gas and particle densities and the relatively small viscosity of gas. Nonetheless, the different treatment may exaggerate the difference between Model A and Model B too. Therefore, to make the results comparable, the same initial packing state should be used, and the acceleration term should be added to both models or none of them.

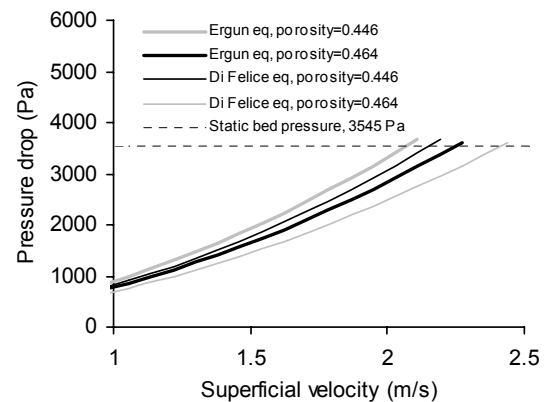


Figure 6 Pressure drop as a function of superficial velocity at two initial packing porosities

Kafui et al. (2002) also showed a significant difference in the pressure drop-superficial gas velocity profiles in the fixed bed regime. Corresponding to which, there is a significant difference in minimum fluidisation velocity. These authors used this result to support their conclusion that the PGF (Model A) is better. However, a careful check of their results shows that there is a problem in validating the simulated pressure drop. In their simulation, the formulation used to calculate particle fluid interaction force is from the Di Felice correlation, but the empirical correlation used to validate the simulated pressure drop is from the Ergun equation. The value calculated from the Di Felice correlation is not equal to that from Ergun equation as shown in Figure 1. The value calculated from the Ergun equation is comparable to that from the Di Felice equation only at porosity 0.4, and the difference increases with the

increase of porosity with the Ergun equation giving a larger value. This will produce a difference in pressure drop as shown in Figure 6, and hence a difference in minimum fluidisation velocity. This difference, however, can only be used to assess the accuracy of the two correlations but not the relative reasonableness of Model A and Model B.

Bi-sized system

Comparison between Model A and Model B is further conducted for bi-sized particle systems with the parameters as listed in table 3. Spherical particles are used as the solid phase fluidized in a rectangular bed. In our previous work (Feng et al, 2001), periodical boundary conditions are applied to the front and rear walls in order to effectively reduce the effect imposed by the front and rear walls and to allow the three-dimensional motion of particles in the bed with a relatively small number of particles. Here, for the convenience of comparison with experiment, the front and rear wall is added to support particles. The flow of gas is assumed to be two-dimensional considering that the bed width is much larger than its thickness.

Solid phase		
Density (kg/m^3)		2,500
Young's Module (N/m^2)		1.0×10^7
Poisson ratio (Nm^{-1})		0.33
Friction coefficient (-)		0.33
Damping coefficient (-)		0.3
Diameter (m)	Flotsam	0.001
	Jetsam	0.002
Particle numbers (-)	Flotsam	22,223
	Jetsam	2,777
Gas phase		
Viscosity ($\text{kgm}^{-1}\text{s}^{-1}$)		1.8×10^{-5}
Density (kg/m^3)		1.205
Bed height (m)		0.26
Bed width (m)		0.065
Bed thickness (m)		0.0082
Cell width (m)		0.005
Cell height (m)		0.005

Table 3 Parameters used for binary-sized systems

A simulation is started with the random generation of particles without overlaps in the rectangular bed, followed by a gravitational settling process for 0.6 seconds. Then, gas is injected at the bottom uniformly to fluidize the bed. The top surface of the packed particles after settling is about 65 mm high, almost the same as the bed width.

Figure 7 shows the solid flow patterns simulated under both model formulations when the gas injection velocity is 1.3 m/s. For better visualization, only particles whose centre points are between 1.5 mm and 2.5 mm in the thickness direction are shown. Less segregation happens for Model A (see Figure 7 A) than Model B (see Figure 7 B).

The difference between Model A and Model B simulations can be further quantified in terms of Lacey mixing index (Lacey, 1954) which is widely used for the study of the mixing kinetics. Its interpretation for this study can be found from our previous publication (Feng et al, 2001). Figure 8 shows the variation of mixing index with time when the gas injection velocity is 1.3 m/s. The

mixing index has a value near one at the initial well-mixed packing state and decreases quickly for the Model B simulation due to the segregation process. After about 20 seconds, it fluctuates around a certain value (0.11 on average), reaching a dynamically stable state. While from the Model A simulation, the value decreases slowly and reaches a value of 0.65 when a dynamically stable state is reached.

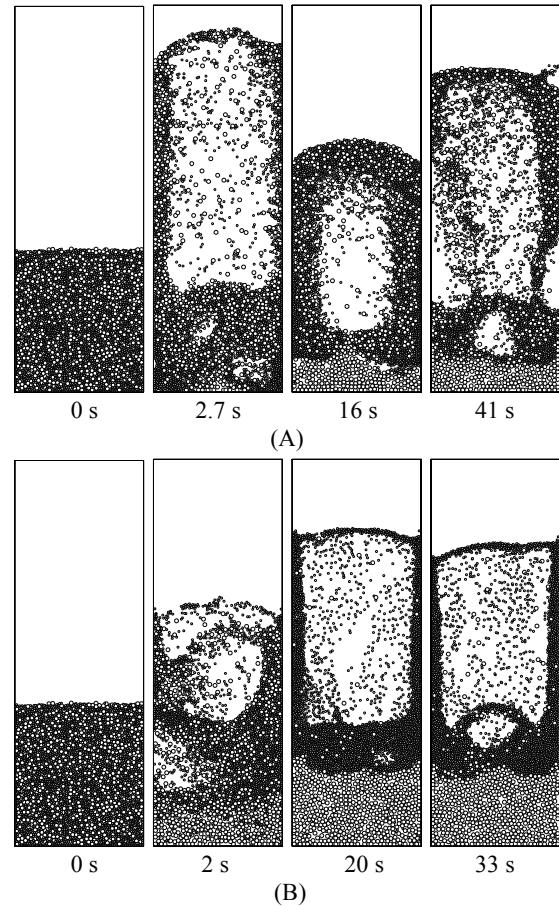


Figure 7 Solid flow patterns at different times when gas injection velocity is 1.3 m/s: A), Model A; B), Model B.

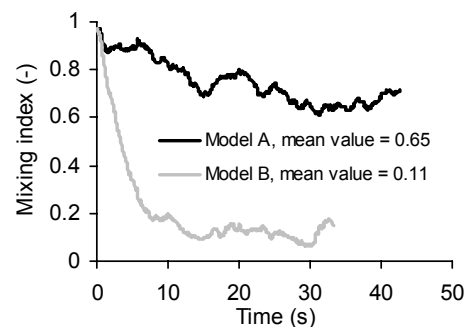


Figure 8. Variation of mixing index with time when the gas injection velocity is 1.3 m/s.

Physical experiments have been conducted under conditions comparable to those used in the simulation. The bed thickness is also 4 times the jetsam diameter. The wall is made of Perspex sheet. Glass beads of diameters 1 and 2 mm are used as the packing/fluidized materials. A segregation/mixing process is recorded by a digital video camera. Different sized particles can be identified by the

colours reflected through light (dark for flotsam and bright for jetsam). Figure 9 shows the solid flow patterns observed where significant segregation happens which close to the simulation of Model B.

At a high velocity, say 1.6 m/s in this study, the flow patterns from Model A and Model B simulation, as well as from experiment at their macroscopically equilibrium state are shown in Figure 10. Both model simulations produce a vigorous particle motion, however, a difference can still be seen. Model A gives less segregation than Model B in the bottom of the bed. Experimental result again shows a preference of the Model B simulation (Figure 10 c).

The difference between Model A and Model B simulation must be related to the different particle-fluid interaction forces caused by different models as shown in Eqs. 5a and 5b, which need to be quantified in the future work. Also, current comparison is qualitatively based on flow pattern, quantitative comparison between experiment and simulation is necessary to fully assess the two model formulations.

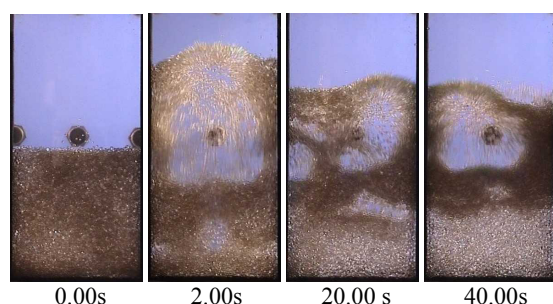


Figure 9 Solid flow patterns observed in the experiment when gas injection velocity is 1.3 m/s

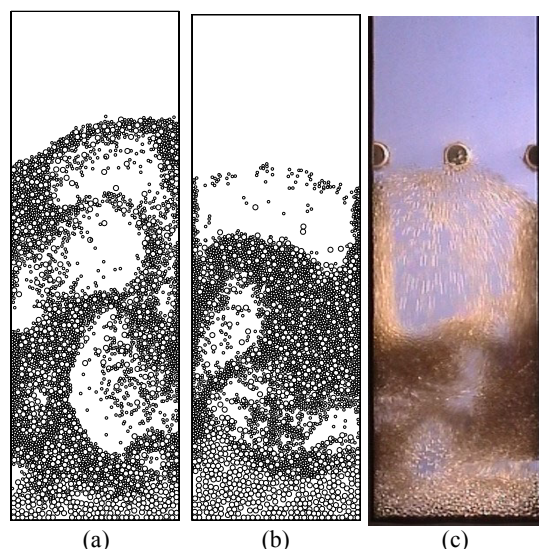


Figure 10 Solid flow patterns at gas velocity 1.6 m/s at their equilibrium state: a) Model A; b) Model B; c) experiment.

CONCLUSIONS

The effect of model formulations on the fluidization behaviour of gas solid flow has been studied through a numerical simulation of mono-sized and bi-sized systems. The simulation results show little difference for mono-sized systems, but a significant difference for bi-sized

systems. Physical experiment shows a preference of Model B. However, further studies are necessary in order to find out the underlying mechanisms and clarify this important matter fully.

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