

Comparison of continuum models using the kinetic theory of granular flow with discrete particle models and experiments: Extent of particle mixing induced by bubbles

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Abstract

The bubble formation and extent of particle mixing induced by a single bubble injected in a mono-disperse fluidised bed at incipient fluidisation conditions has been studied with a Two-Fluid continuum Model (TFM) using the Kinetic Theory of Granular Flow (KTGF) and compared with experiments and simulation results obtained from a Discrete Particle Model (DPM). The effect of different gas-particle drag models and frictional viscosity models on the bubble behaviour and extent of particle mixing has been assessed. To describe the extent of particle mixing well, a frictional viscosity model needs to be included, however, the currently available frictional viscosity models need further improvement.

Introduction

In many industrial multi-disperse gas-solid fluidised bed applications, for example in gas-phase polymerisation reactors or in granulation processes, the particle size distribution and the particle residence time distribution - and hence the particle properties - are largely determined by the rate of segregation of the larger particles and the rate of mixing induced by the movement of the bubbles. Therefore, to describe the particle mixing a fundamental understanding of the influence of the bubble characteristics and bubble dynamics is necessary. With fundamental hydrodynamic models the mixing and segregation behaviour of these type of gas-solid contactors can be studied in great detail.

To describe the hydrodynamics of dense gas-solid fluidised beds on the one hand Discrete Particle Models (DPM) and on the other hand Two-Fluid continuum models (TFM) have been developed. In the DPM (an Euler-Lagrange model) the gas phase is treated as a continuum and every particle is tracked individually, where a detailed collision model is used to account for non-ideal particle-particle or particle-wall interactions. Recently, the DPM has been validated extensively with dedicated experiments using the Particle Image Velocimetry (PIV) technique [1]. The extent of mixing induced by a single bubble injected in a mono-disperse fluidised bed at incipient fluidisation conditions was studied. With a new drag model proposed by Koch&Hill [7] - based on Lattice-Boltzmann simulations - the DPM simulation results improved considerably regarding the bubble size and induced particle mixing compared with the experimental results. Furthermore, also the segregation rates in a bi-disperse freely bubbling fluidised bed were simulated with the DPM and the results matched the experimentally obtained segregation rates quite well. However, the maximum number of particles that can be modelled with the DPM is

less than typically $\pm 1.0 \cdot 10^5$, whereas the number of particles that are present in an industrial fluidised bed is orders of magnitude higher. Therefore, continuum models (Euler-Euler models), where the gas phase and the solid phase are both treated as interpenetrating continua, have been developed to model industrial scale fluidised beds, where the Kinetic Theory of Granular Flow (KTGF) is used to describe the solids phase rheology. Although the continuum models have been studied extensively in the literature (e.g. [4,5,8,11]), these models still lack the capability of describing quantitatively particle mixing and segregation rates in multi-disperse fluidised beds. To understand the short-comings of the continuum models, the DPM can be used as a research-tool in order to validate the underlying assumptions in the TFM.

As a first step in better understanding the mixing and segregation behaviour of multi-disperse fluidised beds, in this work the mixing induced by a single bubble injected in a mono-disperse fluidised bed at incipient fluidisation conditions is studied. The model predictions by the TFM are compared with the DPM simulation results and experiments. Especially the effect of sub-grid scale models, i.e. gas-particle drag and particle-particle interactions, on the bubble formation and the extent of particle mixing in the fluidised bed is investigated.

CFD modelling

Two-fluid continuum model

The Two-Fluid continuum model describes both the gas phase and the solids phase as fully interpenetrating continua using a generalised form of the Navier-Stokes equations for interacting continua (see Table 1). To describe the particle-particle interactions the Kinetic Theory of Granular Flow is used, which expresses the isotropic and deviatoric parts of the solids stress tensor (i.e. the solids pressure and solids shear rate) as a function of the granular temperature, defined as:

$$\theta = \frac{1}{3} \langle \vec{C}_p \cdot \vec{C}_p \rangle \quad (1)$$

where \vec{C}_p represents the particle fluctuation velocity. The derivation of these constitutive equations are discussed in the books by Chapman and Cowling [2] and Gidaspow [4] and the papers by Jenkins and Savage [6], Ding and Gidaspow [3] and Nieuwland et al. [10]. In this work the constitutive equations by Nieuwland et al. have been used for the particle phase rheology.

Discrete Particle Model

In the discrete particle model (DPM) every particle is tracked individually using Newton's second law of motion:

$$m_p \frac{d\vec{v}_p}{dt} = m_p \vec{g} + \frac{V_p \beta}{(1 - \epsilon_g)} (\vec{u} - \vec{v}_p) - V_p \nabla p \quad (2)$$

The gas phase hydrodynamics are solved with the volume-averaged Navier-Stokes equations, given by

$$\frac{\partial(\epsilon_g \rho_g)}{\partial t} + \nabla \cdot \epsilon_g \rho_g \vec{u} = 0 \quad (3)$$

$$\frac{\partial(\epsilon_g \rho_g \vec{u})}{\partial t} + \nabla \cdot \epsilon_g \rho_g \vec{u} \vec{u} = -\epsilon_g \nabla p - \nabla \cdot \epsilon_g \vec{\tau}_g - \vec{S}_p + \epsilon_g \rho_g \vec{g} \quad (4)$$

with \vec{S}_p the source term that accounts for the momentum exchange between the gas and the solids phase:

$$\vec{S}_p = \frac{1}{V} \int \sum_{k=0}^{N_{part}} \frac{V_{p,k} \beta}{1 - \epsilon_g} (\vec{u} - \vec{v}_{p,k}) \delta(\vec{r} - \vec{r}_{p,k}) dV \quad (5)$$

Table 1
Two Fluid Model, governing equations

Continuity equations:

$$\frac{\partial}{\partial t}(\epsilon_g \rho_g) + \nabla \cdot (\epsilon_g \rho_g \vec{u}_g) = 0 \quad (1.1)$$

$$\frac{\partial}{\partial t}(\epsilon_s \rho_s) + \nabla \cdot (\epsilon_s \rho_s \vec{u}_s) = 0 \quad (1.2)$$

Momentum equations:

$$\frac{\partial}{\partial t}(\epsilon_g \rho_g \vec{u}_g) + \nabla \cdot (\epsilon_g \rho_g \vec{u}_g \vec{u}_g) = -\epsilon_g \nabla p_g - \nabla \cdot (\epsilon_g \overline{\overline{\tau}}_g) - \beta(\vec{u}_g - \vec{u}_s) + \epsilon_g \rho_g \vec{g} \quad (1.3)$$

$$\frac{\partial}{\partial t}(\epsilon_s \rho_s \vec{u}_s) + \nabla \cdot (\epsilon_s \rho_s \vec{u}_s \vec{u}_s) = -\epsilon_s \nabla p_s - \nabla \cdot (\epsilon_s \overline{\overline{\tau}}_s) - \nabla p_s + \beta(\vec{u}_g - \vec{u}_s) + \epsilon_s \rho_s \vec{g} \quad (1.4)$$

Granular temperature equation:

$$\frac{3}{2} \left[\frac{\partial}{\partial t}(\epsilon_s \rho_s \theta) + \nabla \cdot (\epsilon_s \rho_s \theta \vec{u}_s) \right] = -(p_s \overline{\overline{I}} + \epsilon_s \overline{\overline{\tau}}_s) : \nabla \vec{u}_s - \nabla \cdot (\epsilon_s q_s) - 3\beta\theta - \gamma \quad (1.5)$$

Gas-particle interaction: Drag model

The interphase momentum exchange coefficient β in both the TFM and the DPM is usually calculated with a combination of the well-known Ergun equation at low gas porosities and the Wen&Yu equation at high gas porosities. However, recently Lattice-Boltzmann simulations have shown large discrepancies for the gas-particle drag at intermediate gas porosities. A comparison between DPM calculations of a single bubble in a mono-disperse fluidised bed and experiments showed that the Ergun and Wen&Yu equations overpredicted the bubble size considerably [1] and that better results were obtained with a drag model proposed by Koch&Hill based on Lattice-Boltzmann simulations [7].

Particle-particle interactions: Frictional stress model

At high particle volume fractions, the momentum transfer in the particulate phase becomes dominated by long-term and multi-particle contacts, which are not accounted for in the KTGF. To be able to model these dense regions with continuum models, an additional term is added to the shear viscosity, the so-called frictional viscosity. Laux [9] tested several models from the field of soil mechanics and the frictional viscosity term that gave the best results, is given by:

$$\mu_{s,fric} = \frac{6 \sin \phi_I}{9 - \sin^2 \phi_I} \frac{3\sqrt{2} |(\lambda_s \nabla \cdot \vec{u}_s - \frac{p_s}{\epsilon_s})|}{2\sqrt{3} \sqrt{\overline{\overline{D}}_{ij} : \overline{\overline{D}}_{ij}}} \quad (6)$$

where ϕ_I is the internal angle of friction and the rate of strain tensor $\overline{\overline{D}}_{ij}$ is given by:

$$\overline{\overline{D}}_{ij} = \frac{1}{2} \left((\nabla \vec{u}_s) + (\nabla \vec{u}_s)^T \right) - \frac{1}{3} \nabla \cdot \vec{u}_s \overline{\overline{I}} \quad (7)$$

Lately, Srivastava and Sundaresan [12] presented a frictional viscosity model that is given by:

$$\mu_{s,fric} = \frac{p_c(\epsilon_s) \sqrt{2} \sin \phi_I}{2\epsilon_s \sqrt{(\overline{\overline{D}}_{ij} : \overline{\overline{D}}_{ij} + \psi \theta_s / d_p^2)}} \quad (8)$$

Table 2

Base case settings for DPM and TFM calculations for a single bubble injected in a mono-disperse fluidised bed at incipient fluidisation conditions.

| | DPM | TFM |
|-------------------------------------|------------------------|-----------------------|
| width | 15 cm | 15 cm |
| height | 45 cm | 60 cm |
| depth | 1.5 cm | - |
| bedheight at u_{mf} | 22 cm | 30 cm |
| number of grid cells in x-direction | 15 | 30 |
| number of grid cells in y-direction | 1 | - |
| number of grid cells in z-direction | 45 | 60 |
| time step | $1.0 \cdot 10^{-4}$ s | $1.0 \cdot 10^{-5}$ s |
| number of particles | 30000 | - |
| collision model | Soft-sphere | KTGF |
| normal spring stiffness | 20000 | - |
| tangential spring stiffness | 5714 | - |
| background velocity | 1.2 m/s | |
| jet pulse velocity | 20 m/s | |
| jet pulse duration | 150 ms | |
| particle density | 2526 kg/m ³ | |
| particle diameter | $2.5 \cdot 10^{-3}$ m | |
| coefficient of restitution | 0.97 | |
| drag model | Koch&Hill | |

$$p_c(\epsilon_s) = \begin{cases} F \frac{(\epsilon_s - \epsilon_{s,min})^r}{(\epsilon_{s,max} - \epsilon_s)^s} & \epsilon_s > \epsilon_{s,min} \\ 0 & \epsilon_s < \epsilon_{s,min} \end{cases} \quad (9)$$

where F , r , s and ψ are constants, with the values $F = 0.05N/m^2$, $r = 2$, $s = 5$ and $\psi=1$. The main difference between these frictional viscosity models is the additional term $(\psi\theta_s/d_p^2)$ in the denominator of the viscosity model proposed by Srivastava and Sundaresan to account for strain rate fluctuations. Furthermore, Srivastava and Sundaresan use the critical state pressure (p_c) instead of the solids pressure (p_s) obtained from the KTGF in the calculation of the frictional viscosity and this critical state pressure is also added to the solids pressure when calculating the solids pressure gradient in the solids phase momentum equation.

Comparison of the TFM with the DPM and experiments

The bubble formation and the particle mixing induced by a single bubble injected in a mono-disperse fluidised bed at incipient fluidisation conditions has been studied with the TFM and compared with the DPM simulation results and experiments. The effect of the different drag models and frictional viscosity models has been investigated.

Bubble formation

The bubble size of a single bubble injected in a mono-disperse fluidised bed at 0.2 s after injection predicted by the TFM are compared with DPM simulation results and experiments in Figure 1. The drag model proposed by Koch&Hill predicts a smaller bubble size and a more pronounced 'raining' of the particles through the roof of the bubble compared to the drag model by Ergun/Wen&Yu for both the DPM (compare snapshots (b) and (c)) and the TFM (compare

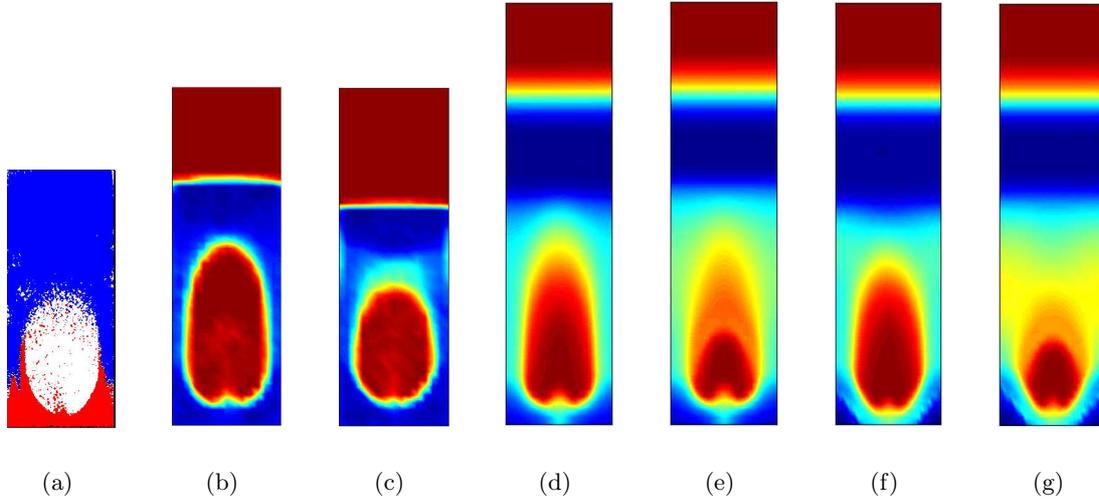


Figure 1. Snapshots of the bubble in a mono-disperse fluidised bed at 0.2 s after injection: Comparison between TFM with DPM and experiments; (a) Experiment; (b) DPM with Ergun/Wen&Yu; (c) DPM with Koch&Hill; (d) TFM with Ergun/Wen&Yu; (e) TFM with Koch&Hill; (f) TFM with Ergun/Wen&Yu and Laux; (g) TFM with Koch&Hill and Laux.

(d) and (e), (f) and (g)), which compares better with the experimental results [1]. The effect of the different drag models on the bubble size and the raining of the particles is somewhat larger in the TFM. With the frictional viscosity model by Laux the TFM predicts a somewhat rounder bubble (compare (e) and (g)) due to the increased shear viscosity just above the bubble. The effect of the additional frictional viscosity is more pronounced when using the Koch&Hill drag model. Defining a bubble surface at a gas porosity of 0.85 (the lightest colour in Figure 1), the bubble size and shape predicted by the TFM with the Koch&Hill drag model and Laux' frictional viscosity model (g) compare very well with the experimental results.

Particle mixing

Although the effect of the frictional viscosity on the predicted bubble size and shape by the TFM is moderate, its effect on the particle mixing is very pronounced. The bubble size is mainly determined by the drag exerted on the particles by the gas phase and the mixing of the particles is dominated by particle-particle interactions, especially in the dense regions where sustained multi-particle contacts prevail (friction). In Figure 2 the particle mixing induced by a single rising bubble in a mono-disperse fluidised bed, initially at incipient fluidisation conditions, predicted by the TFM for the different drag models and with and without frictional viscosity is compared with the DPM and experimental results. To study the extent of particle mixing, in the experiment and in the DPM simulations the fluidised bed was initially filled with two layers of particles, differing only in colour. For the TFM simulations tracer particles, initially positioned at regular spacings, were used to visualise the induced particle mixing.

The figure clearly shows that the TFM without a frictional viscosity model largely overpredicts the extent of solids mixing, i.e. the upward transportation of the bottom layer of particles. With the frictional viscosity model by Laux the extent of particle mixing predicted by the TFM compares much better with the experiment and the DPM simulations. With the Ergun/Wen&Yu drag closures both the DPM and the TFM predict a slightly higher particle mixing due to the small overprediction of the bubble size.

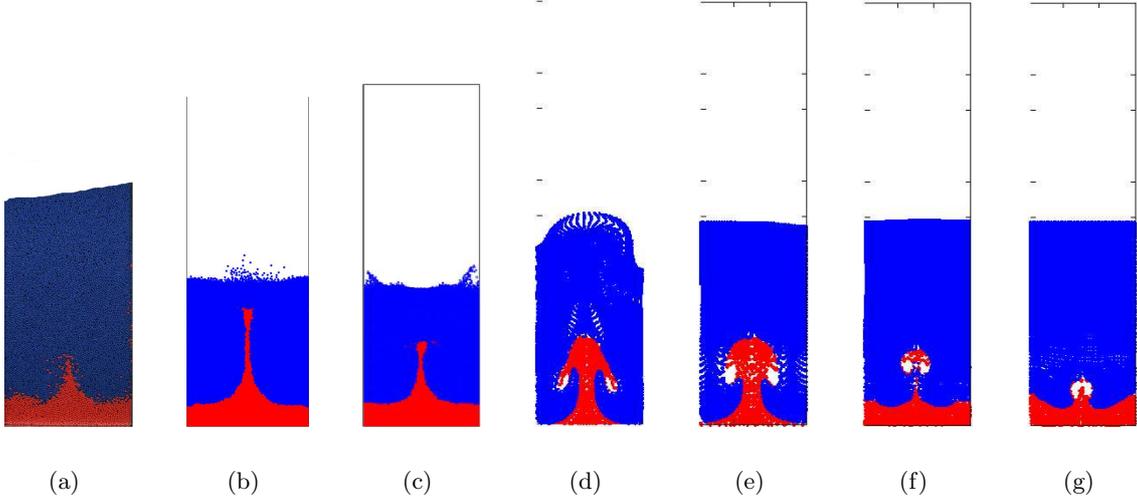


Figure 2. Snapshot of the mono-disperse fluidised bed after a single bubble has passed completely through a bed, initially consisting of two layers of particles differing only in colour. (a) Experiment; (b) DPM with Ergun/Wen&Yu; (c) DPM with Koch&Hill; (d) TFM with Ergun/Wen&Yu; (e) TFM with Koch&Hill; (f) TFM with Ergun/Wen&Yu and Laux; (g) TFM with Koch&Hill and Laux.

Effect of frictional viscosity model

Although the particle mixing and the bubble size and shape was predicted well by the TFM using the Koch&Hill drag model and the frictional viscosity model by Laux for a single bubble injected in a mono-disperse fluidised bed at incipient fluidisation conditions at 0.2 s after injection, the bubble behaviour at longer times is not well captured. In contrast to the experiment and the DPM simulation results, the bubble grew into a slug after 0.3 s after injection, as illustrated in Figure 3. However, the TFM without the frictional viscosity model did maintain the bubble shape for longer times after injection. Therefore, the frictional viscosity model proposed by Srivastava and Sundaresan [12] was tried. In their model the effect of strain rate fluctuations ($\psi\theta_s/d_p^2$) was added to avoid infinite shear viscosities in regions where $\overline{D}_{ij} : \overline{D}_{ij}$ approaches zero. Although Srivastava and Sundaresan propose that the scaling factor ψ is in the order of unity, this factor had to be decreased significantly for the case discussed in this work with relatively large particles to avoid eliminating the frictional viscosity contribution. The TFM using the frictional viscosity model proposed by Srivastava and Sundaresan with $\psi = 0.001$ does not predict slug formation, but the bubble 'dissolves' in the emulsion phase before the bubble can reach the top of the bed. Actually, no differences in the bubble behaviour could be discerned when using different values of ψ . This indicates that the different bubble behaviour is mainly caused by the critical state pressure (p_c) used in the frictional viscosity model by Srivastava and Sundaresan, which is only a function of the solids volume fraction, instead of the solids pressure (p_s) used in the model by Laux. Since the solids pressure is much higher than the critical state pressure, especially in dense regions, the frictional viscosity predicted by the model by Laux is much higher. The much lower frictional viscosity predicted by the TFM with the closures by Srivastava and Sundaresan results in a large overestimation of the extent of particle mixing (comparable to the case without a frictional viscosity model).

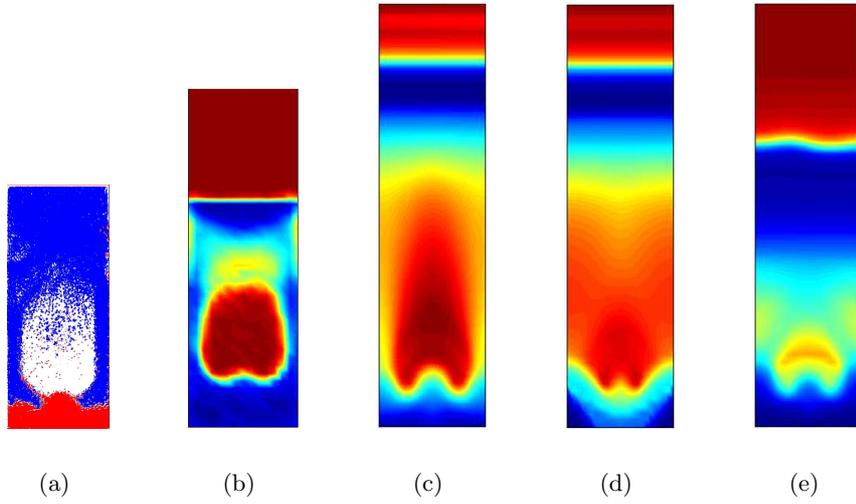


Figure 3. Snapshot of a single bubble in a mono-disperse fluidised bed at 0.3 s after injection. (a) Experiment; (b) DPM; (c) TFM without frictional viscosity model; (d) TFM with Laux; (e) TFM with Srivastava&Sundaresan.

Conclusions

The bubble formation and extent of particle mixing induced by a single bubble injected in a mono-disperse fluidised bed at incipient fluidisation conditions was studied with the TFM with different drag models and frictional viscosity models and compared with experiments and DPM simulation results. With the drag model proposed by Koch&Hill a smaller bubble and more pronounced 'raining' of the particles through the roof of the bubble is predicted compared to the often used drag model by Ergun/Wen&Yu, and when including the frictional viscosity model by Laux a smaller and rounder bubble is calculated, both improving the simulation results in comparison with the experiment. The extent of particle mixing was largely overpredicted by the TFM without a frictional viscosity model. When incorporating the frictional viscosity model by Laux a much better agreement with the experiment was found regarding the particle mixing, however, the bubble grew into a slug, which was not observed in the experiment. With a slightly different frictional viscosity model proposed by Srivastava and Sundaresan no improvements could be obtained for the case considered in this work. Future work is focused on a more detailed study on the particulate phase rheology at high solids volume fractions by means of Euler-Lagrangian simulations.

List of symbols

| | | | |
|-------|--|-------|--|
| C | particle fluctuation velocity, m/s | p_s | particle pressure, Pa |
| C_d | drag coefficient, - | q_s | pseudo Fourier flux of kinetic fluctuating energy, kg/(ms) |
| d | diameter, m | S_p | particle gas momentum exchange, Pa |
| g | gravitational acceleration, m/s ² | u | fluid velocity, m/s |
| m | mass, kg | v | particle velocity, m/s |
| p | pressure, Pa | V | volume, m ³ |
| p_c | critical state pressure, Pa | | |

Greek

| | | | |
|------------|---|-----------|---|
| β | interphase momentum exchange coefficient, $\text{kg}/(\text{m}^3\text{s})$ | λ | bulk viscosity, $\text{kg}/(\text{ms})$ |
| γ | dissipation rate due to inelastic particle-particle collisions, $\text{kg}/(\text{ms}^3)$ | μ | viscosity, Pa s |
| δ | delta function, - | ρ | density, kg/m^3 |
| ϵ | gas fraction, - | τ | stress tensor, Pa |
| θ | granular temperature, m^2/s^2 | ϕ_I | internal angle of friction, - |

Subscripts

| | |
|---|----------|
| g | gas |
| p | particle |
| s | solid |

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