A grid-independent EMMS/bubbling drag model for bubbling and turbulent fluidization

Luo, Hao; Lu, Bona; Zhang, Jingyuan; Wu, Hao; Wang, Wei

Published in:
Chemical Engineering Journal

Link to article, DOI:

Publication date:
2017

Document Version
Peer reviewed version

Link back to DTU Orbit

Citation (APA):
A grid-independent EMMS/bubbling drag model for bubbling and turbulent fluidization

Hao Luo\textsuperscript{a,c}, Bona Lu\textsuperscript{a,b,*}, Jingyuan Zhang\textsuperscript{a,b}, Hao Wu\textsuperscript{c}, We Wang\textsuperscript{a,b,*}

\textsuperscript{a} State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China

\textsuperscript{b} Sino-Danish College, University of Chinese Academy of Sciences, Beijing, 100049

\textsuperscript{c} Department of Chemical and Biochemical Engineering, Technical University of Denmark, 2800 Kongens Lyngby, Denmark

* Corresponding authors. Email addresses: bnlu@ipe.ac.cn (B. Lu), wangwei@ipe.ac.cn (W. Wang).

Abstract

The EMMS/bubbling drag model takes the effects of meso-scale structures (i.e. bubbles) into modeling of drag coefficient and thus improves coarse-grid simulation of bubbling and turbulent fluidized beds. However, its dependence on grid size has not been fully investigated. In this article, we adopt a two-step scheme to extend the EMMS/bubbling model to the sub-grid level. Thus the heterogeneity index, $H_D$, which accounts for the hydrodynamic disparity between homogeneous and heterogeneous fluidization, can be correlated as a function of both local voidage and slip velocity. Simulations over a periodic domain show the new drag model is less sensitive to grid size because of the additional dependence on local slip velocity. When applying the new drag model to simulations of realistic bubbling and turbulent fluidized beds, we find grid-independent results are easier to obtain for high-velocity turbulent fluidized bed cases. The simulation results indicate that the extended EMMS/bubbling drag model is a potential method for coarse-grid simulations of large-
Introduction

Gas-solid fluidization has wide applications in various industries, such as fluid catalytic cracking (FCC), methanol to olefins (MTO), coal gasification and combustion, owing to its advantages in gas-particle contact, heat and mass transfer, and operating flexibility. With the increase of gas velocity, fluidization regime may experience a series of transitions covering homogenous expansion, bubbling fluidization, turbulent fluidization, fast fluidization and pneumatic conveying [1-3]. Different flow regimes are characterized by different meso-scale structures, such as bubbles or voids in bubbling and turbulent fluidization [4, 5], and particle clusters in the so-called fast fluidization [1, 6, 7]. These meso-scale structures are recognized to have big impact on the momentum, heat and mass transfer as well as reactions, thus should be taken into account in modeling.

Of various computational fluid dynamic (CFD) approaches, the Eulerian-Eulerian two-fluid model (TFM) requires the least computational resources, and thus, is widely used for simulating large-scale fluidized bed reactors. However, there are still controversial opinions on the applicability of the local equilibrium assumption underlying the TFM [8-10]. In addition, when the TFM is used with coarse-grid resolution in industrial applications, the grid size could be over one hundred times the particle diameter, as in the cases of Lu et al. [11], Schneiderbauer et al. [12] and Shah et al. [13]. Such coarse-grid resolution, if without sub-grid modeling, may greatly reduce the accuracy of simulation [7, 11, 13, 14].
In recent years, the effect of sub-grid meso-scale structures on the drag has received much attention [1, 15-20]. Among these researches, the energy-minimization multi-scale (EMMS) approach has been found successful in correcting the drag and predicting the flow distribution in circulating fluidized bed (CFB) of fine particles [11, 21-23]. In the EMMS model, the heterogeneous gas-particle flow was characterized by the meso-scale structure consisting of a particle-rich dense phase in form of clusters and a gas-rich dilute phase in form of dispersed particles. Eight parameters ($\varepsilon_{gc}$, $U_{gc}$, $U_{sc}$, $\varepsilon_{gf}$, $U_{gf}$, $U_{sf}$, $f$, $d_{cl}$) were assigned to quantify such meso-scale structure and were closed by six equations including mass and momentum conservations and a stability condition $N_u \rightarrow \min [15]$. To couple the EMMS model with CFD, Yang et al. [24, 25] introduced an acceleration term for both dense and dilute phases and then obtained a structure-dependent EMMS drag. Wang and Li [1] further proposed a two-step scheme called EMMS/matrix, in which the meso-scale parameters ($\varepsilon_{gc}$, $d_{cl}$) were determined at the global reactor scale through solving a set of conservation equations and the stability condition, while the remaining variables were determined in the second step by satisfying local conservation equations within computational cells, thereby the drag correction in term of the heterogeneity index, $H_D = \beta/\beta_0$, was found to be a function of local slip velocity $u_r$ and local voidage $\varepsilon_g$. In contrast, pervious meso-scale models [24, 25] were found to result in heterogeneity index as only a function of voidage. This additional dependence of drag correction on the slip velocity was considered to be critical to reduce the sensitivity of CFD simulation on grid resolution [16, 26]. Indeed some other researches also confirmed that the drag correction should not only depend on voidage but also on slip velocity [19, 26], and such additional dependency on slip velocity was helpful to obtain grid-independent results and improve accuracy [27].
To extend the application of the EMMS model to the realm of bubbling fluidization, Shi et al. [4] and Hong et al. [5] introduced bubbles in place of the particle clusters to characterize the meso-scale structure. This drag model called EMMS/bubbling model improved CFD performance for both bubbling and turbulent fluidized beds [5, 28]. However, its dependence on the grid size has not been fully investigated. In particular, whether this grid dependence can be reduced by introducing the factor of local slip velocity \( U_r \), as in the case of EMMS/matrix drag model, remains to be explored.

In this paper, we aim to introduce the local slip velocity in the EMMS/bubbling model by following the two-step scheme of the EMMS/matrix drag model. Then, a series of simulations are carried out in the 2D periodic domain to test the grid dependence of the new EMMS/bubbling drag model. Finally, this two-step EMMS/bubbling drag model is tested through simulations of a bubbling fluidized bed and two turbulent fluidized beds.

### 2. Extension of EMMS/bubbling model to sub-grid level

#### 2.1 Model derivation

In this work, we try to develop a new drag model based on the work of Hong et al. [5]. In the EMMS/bubbling model [5], monodisperse gas-solid flow is resolved into a dense phase (emulsion, denoted by subscript c) and a dilute phase (bubble, denoted by subscript f). There are seven equations and a stability condition to close ten variables, i.e., \( U_{gc}, U_{sc}, a_{sc} \) and \( \varepsilon_{gc} \) for the dense phase, \( U_{gf}, U_{sf}, a_{sf} \) and \( \varepsilon_{gf} \) for the dilute phase and \( f \) and \( d_b \) for the interphase.

The momentum balance equations for the dense phase and inter-phase, and dilute phase are as
follows

$$fF_{dc} + F_{d_b} = \frac{3}{4} C_{dc} \frac{f(1-\varepsilon_{dc})}{d_p} \rho_c U_{rc}^2 + \frac{3}{4} C_{db} \frac{1-f}{d_b} \rho_b U_{rb}^2 = f (1-\varepsilon_{dc}) (\rho_s - \rho_g) (g + a_{sc}) \cdot (1)$$

$$F_{df} = \frac{3}{4} C_{df} \frac{1-\varepsilon_{df}}{d_p} \rho_b U_{rB}^2 = (1-\varepsilon_{df}) (\rho_s - \rho_g) (g + a_{df}) \cdot (2)$$

Pressure balance of different phases [5],

$$F_{df} + \frac{F_{df}}{1-f} = F_{dc} \cdot (3)$$

The mass balances for the gas and solid phases require that

$$U_g = fU_{gc} + (1-f)U_{gf} \cdot (4)$$

$$U_s = fU_{sc} + (1-f)U_{st} \cdot (5)$$

The mean voidage is related to the dense-phase and dilute-phase voidages by

$$\varepsilon_g = f \varepsilon_{dc} + (1-f) \varepsilon_{df} \cdot (6)$$

The bubble diameter, as in our previous work, follows the correlation of Horio and Nonaka [29],

which was reported applicable to a variety of powders [29-32].

$$d_b = \left[ -\gamma_m + \left( \gamma_m^2 + 4d_{bm}/D_t \right)^{0.5} \right]^{1/2} D_t/4 \cdot (7)$$

where

$$\gamma_m = 0.0256 (D_t/g) / U_{mf} \cdot d_{bm} = 2.59 g^{-0.2} \left[ (U_g - U_{gc}) \pi D_t^2 / 4 \right]^{0.4} \cdot (8)$$

The above equations are assumed to satisfy the stability condition in term of the minimization

of normalized $N_{st}$, the mass-specific energy consumption rate for suspending particles, as follows:

$$\frac{N_{st}}{N_{st}} = \left( \frac{fF_{dc} U_{gc} + (1-f) F_{df} U_{df}}{(1-\varepsilon_g) \rho_s + (1-f) \varepsilon_{df} U_g / \rho_g} \right) \left( 1 - \frac{\rho_s - \rho_g}{\rho_s} \frac{gU_g}{\rho_e} \right) \to \text{min} \cdot (9)$$

Table 1 Summary of parameters and definitions in EMMS/bubbling model (adapted from Hong et
### Characteristics

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Dilute phase</th>
<th>Dense phase</th>
<th>Inter-phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter</td>
<td>$d_p$</td>
<td>$d_p$</td>
<td>$d_b$</td>
</tr>
<tr>
<td>Voidage</td>
<td>$\varepsilon_{gf}$</td>
<td>$\varepsilon_{gc}$</td>
<td>1-$f$</td>
</tr>
<tr>
<td>Superficial relative</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Velocity: $U_{st} = U_{stf} - \frac{U_d \varepsilon_{df}}{\varepsilon_{df}}$</td>
<td>$U_{sc} = U_{sc} - \frac{U_d \varepsilon_{df}}{\varepsilon_{df}}$</td>
<td>$U_{in} = f(U_t - U_c)$</td>
<td></td>
</tr>
<tr>
<td>Reynolds number: $Re_i = \frac{\rho_d d_i U_{stf}}{\mu}$</td>
<td>$Re_c = \frac{\rho_d d_c U_{sc}}{\mu}$</td>
<td>$Re = \frac{\rho_d d_c U_{stf}}{\mu}$</td>
<td></td>
</tr>
</tbody>
</table>
| Standard drag coefficient: $C_{d0} = \frac{24}{Re_i^{0.313}} + \frac{3.6}{Re_i^{0.313}}$ | $C_{d0} = \frac{24}{Re_c^{0.313}} + \frac{3.6}{Re_c^{0.313}}$ | \[
\left\{
\begin{align*}
C_{d0} &= 38Re_i^{-0.5} & (0 < Re_i \leq 1.8) \\
C_{d0} &= 2.7 + \frac{24}{Re_i} & (Re_i > 1.8)
\end{align*}
\right.
\] |
| Effective drag coefficient: $C_{df} = C_{d0} \cdot 0.65$ | $C_{df} = C_{d0} \cdot 0.65$ | $C_{df} = C_{d0} \cdot 0.65$ |
| Number density: $m_i = \frac{1 - \varepsilon_{gf}}{\pi d_{i}^3/6}$ | $m_c = \frac{1 - \varepsilon_{gc}}{\pi d_{c}^3/6}$ | $m_i = \frac{1 - f}{\pi d_{b}^3/6}$ |
| Drag force on each particle or bubble: $F_i = C_{df} \frac{\pi d_{b}^2 \rho_d U_{stf}^2}{4}$ | $F_i = C_{df} \frac{\pi d_{c}^2 \rho_d U_{sc}^2}{2}$ | $F_i = C_{df} \frac{\pi d_{b}^2 \rho_d U_{stf}^2}{2}$ |
| Drag force in unit volume: $F_{df} = m_i F_i$ | $F_{df} = m_i F_i$ | $F_{df} = m_i F_i$ |

* The mean velocities of the dilute and dense phases are defined as $U_t = (\rho_d U_{stf} + \rho_s U_{set})/\rho_b$ and $U_c = (\rho_c U_{set} + \rho_s U_{sc})/\rho_c$, respectively, where $\rho_b$, $\rho_c$ and $\mu_c$ are expressed as $\rho_b = \varepsilon_{gf} \rho_d + \varepsilon_{df} \rho_s$, $\rho_c = \varepsilon_{gc} \rho_c + \varepsilon_{sc} \rho_s$, and $\mu_c = \mu_0 [1 + 2.5 \varepsilon_{gc} + 10.05 \varepsilon_{gc}^2 + 0.00273 \exp(16.6 \varepsilon_{gc})]$, respectively.

The related definitions and model parameters are summarized in Table 1. Similar to the two-step scheme of the EMMS matrix drag model, in the first step, we calculate the meso-scale structure parameters ($\varepsilon_{gc}$, $d_b$) by solving the set of conservation equations and the stability condition,
Eqs.(1) to (8) at the reactor level under the given superficial gas velocity. The scheme for this first step is referred to Hong et al [5]. $\varepsilon_{gc}$ and $d_b$ can thus be expressed as a function of voidage. As indicated in the EMMS/matrix model, the voidage in bubbles tends to $\varepsilon_{max}$ ($\varepsilon_{max}$=0.9997) and $a_{sf}$ tends to $-g$. Then, the remaining variables, i.e. $(U_{gc}, U_{sc}, a_{sc}, f)$ for the dense phase and $(U_{gf}, U_{sf})$ for the dilute phase, can be determined in the second step by solving the conservation equations (Eqs. (1) ~ (6)) locally within each grid. As indicated in Lu et al. [16], the velocities $U_{gc}, U_{sc}, U_{gf}, U_{sf}$ can be further reduced to two slip velocities $(U_{ri}, U_{rc})$ by combining the definitions of superficial velocities as shown in Table 1 and the equations (Eqs.(4) ~ (6)). The relationship between two slip velocities $(U_{ri}, U_{rc})$ can be expressed as Eq. (9),

$$U_{ri} = \frac{f \left( 1 - \varepsilon_g \right)}{\left( 1 - f \right) \left( \varepsilon_g - \varepsilon_s \right)} \left( U_t - f U_{rc} - \frac{\rho_g \left( 1 - f \right) \left( \varepsilon_g - \varepsilon_s \right)}{\rho_c \left( 1 - \varepsilon_g \right)} U_{rc} \right).$$

(9)

The detailed derivation of Eq.(9) is provided in Supplementary material. Finally, four unknown parameters $(f, U_{rc}, U_{ri}, a_{sc})$ in the second step are closed by four equations, Eqs. (1), (3), (6) and (9).

With the meso-scale parameters ($\varepsilon_{gc}, d_b$) resolved in the first step, the scheme of the second step is described as follows:

(1) traverse over trial values of local parameters, $U_t$ and $\varepsilon_g$,

(2) calculate the volume fraction of dense phase $f$ from Eq. (6),

(3) calculate $U_{rc}$ and $U_{ri}$ from Eq. (3) and Eq. (9),

(4) calculate $a_{sc}$ from Eq. (1).

Through above four steps, all parameters are solved and the structure-dependent drag coefficient are obtained as follows.

2.2 Structure-dependent drag coefficient
As in the work of Hong et al. [5], the structure-dependent drag coefficient is determined by

$$\beta = \frac{\varepsilon_g^2}{U_r} \left[ f F_{dc} + (1 - f) F_{df} + F_{dn} \right]$$

$$= \frac{\varepsilon_g^2}{U_r} \left( \rho_s - \rho_g \right) \left[ f \left(1 - \varepsilon_{gc}\right) \left(g + a_{sc}\right) + (1 - f) \left(1 - \varepsilon_{gf}\right) \left(g + a_{sf}\right) \right]$$

(10)

And the heterogeneity index, $H_D$, is defined by

$$H_D = \frac{\beta}{\beta_0},$$

(11)

where

$$\beta_0 = \frac{3}{4} C_{\alpha_0} \varepsilon_g \frac{1 - \varepsilon_g}{d_p} \rho_s |u_g - u| \varepsilon_g^{-2.65}.$$

Because of the two-step scheme, as in Lu et al. [16], the heterogeneity index, $H_D$, can be also expressed as a function of local slip velocity ($\text{Re}= U_r \rho_s d_p / \mu_g$) and voidage. As shown in Fig.1, The drag coefficient is much less than the homogenous one within most of the voidage range, except near the two ends corresponding to the packed state and extremely dilute flow, respectively. Higher slip velocity generally results in higher values of $H_D$, and the previous version of EMMS/bubbling drag (Hong et al. [5]) can thus be viewed as a particular case of this work when the local superficial slip velocity $U_r$ is equal to the global superficial slip velocity ($U_g - G_\delta \varepsilon_g / \rho_g \mu_g$). To facilitate its coupling with CFD code, $H_D$ is fitted in the form of

$$H_D = a \text{Re}^{b (\text{Re} + c)},$$

where $a$, $b$, and $c$ are all functions of voidage.
Fig. 1 The heterogeneity index ($H_D$) of (a) new EMMS/bubbling model for a bubbling fluidized bed and its comparison with that of (b) Hong et al. [5] (Dubrawski et al. [33]: $\rho_g=1.225$ kg/m$^3$, $\rho_p=1560$ kg/m$^3$, $d_p=103$ $\mu$m, $\mu_g=1.8\times10^{-5}$ Pa$\cdot$s, $U_g=0.5$ m/s, $\varepsilon_{mf}=0.45$, $G_s=0$, $D_t=0.133$)

3 Sensitivity to grid size

3.1 Simulation settings

The grid size has significant effects on the simulation results [7, 19, 34]. To test the grid dependence when applying the new drag model, we chose a 2D doubly periodic domain with dimension comparable to a typical coarse grid in TFM simulations, as in the work of Lu et al. [16] and Agrawal et al. [7].

Square grids were generated uniformly by using Gambit® 2.4, and ANSYS Fluent® 15 was used as the CFD solver. Two different solid concentrations, i.e., $\varepsilon_s=0.05$ and $\varepsilon_s=0.2$, were adopted to represent the dilute and dense flow. Fine particles were distributed uniformly in the domain at the beginning. The pressure drop in the vertical direction was specified to be equal to the gravity of solid particles. Both gas and solid phases were initialized with zero velocity and then a perturbation was introduced. Following many previous researches, to mention but a few, Agrawal et al. [7], Igci et al. [34], and Lu et al. [16], the time series of slip velocity of y-direction were monitored to
observe its fluctuation. After a period of time, the quasi-steady state was reached where the
time-averaged slip velocity kept almost unchanged, then statistical analysis could be started to
determine the time-averaged quantities. In this study, all simulations over the periodic domain ran
for 8 seconds and the last 4 seconds were collected for time-averaged statistics. Implicit formulation
was adopted to solve the volume fraction equation, since it reached pseudo-steady state faster than
explicit formulations [35]. The physical time step $2 \times 10^{-4}$ s chosen in present work was based on the
work of Lu et al [16]. However, for the case of the finest grid (128×512), using such a time step
causes convergence difficulty, thus, a smaller physical time step $5 \times 10^{-5}$ s was chosen. The
Favre-averaged slip velocity over the domain, as applied in Agrawal et al. [7], was used to quantify
the effects of meso-scale structure on the drag, and defined by

$$
\overline{u_i} = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{E_{g(i)}s_{g(i)}}{\varepsilon_g} - \frac{E_{s(i)}s_{s(i)}}{\varepsilon_s} \right),
$$

(12)

Where $N$ is the number of cells. More simulations settings are shown in Table 2 and the drag
formulations are provided in Table B.2 of Supplementary material. Although the correction of this
work is complicated, the computational time does not increase too much as they only involve
algebraic calculation. According to our experience, the simulation time of using the model of
Hong et al. [5] and this work are almost the same.

Table 2 Parameters settings for simulations in a periodic domain.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle diameter, µm</td>
<td>97</td>
</tr>
<tr>
<td>Particle density, kg/m³</td>
<td>1500</td>
</tr>
<tr>
<td>Gas density, kg/m³</td>
<td>0.6747</td>
</tr>
<tr>
<td>Gas viscosity, Pa·s</td>
<td>$2.7782 \times 10^{-5}$</td>
</tr>
<tr>
<td>Domain size, mm²</td>
<td>25×100</td>
</tr>
<tr>
<td>Number of grids</td>
<td>4×16, 8×32, 16×64, 32×128, 64×256, 128×512</td>
</tr>
</tbody>
</table>
Restitution coefficient 0.9

Drag coefficients Hong et al. [5]/This work.

Physical time-step $2 \times 10^{-4}$ s, $5 \times 10^{-5}$ s

3.2 Results and discussions

Fig. 2 shows the variation of time-averaged axial slip velocity against grid size for two solid concentrations. To the left of the figure, the y-coordinates are scaled with the terminal velocity of a single particle ($u_t=0.255$ m/s), and to the right, y-coordinates are scaled with the time-averaged slip velocity of the coarsest-grid case ($6.25 \times 6.25$ mm$^2$). X-abscissas are scaled with the particle diameter, $d_p$.

For the case of $\varepsilon_s=0.05$, the slip velocities keep changing until the grid size decreases to $4d_p$.

During grid refinement, the dimensionless slip velocity ($u_r/u_t$) predicted by using the drag of Hong et al. [5] changes from three to five. By comparison, the change predicted by using our new drag is much smaller.

For the case of $\varepsilon_s=0.2$, the slip velocity predicted by using the drag of Hong et al. [5] converges to its asymptotic value again at the grid size of about $4d_p$, whereas the sensitivity to the grid size is weaker compared to the dilute flow case ($\varepsilon_s=0.05$). And our new drag model shows even weaker dependence on the grid size. That implies a coarser grid could be applied when using our new drag based on two-step scheme.
Fig. 2 Effect of grid resolution on time-averaged axial slip velocity with snapshots of solids distribution. $u_r^*$ is the time-averaged axial slip velocity over the largest grid scheme for each case in simulations. The drag coefficients of EMMS/bubbling model and this work are based on the following operating conditions ($\rho_g=0.6747$ kg/m$^3$, $\rho_p=1500$ kg/m$^3$, $d_p=97$ $\mu$m, $\mu_g=2.7782\times10^{-5}$ Pa·s, $\varepsilon_{mf}=0.4$, $U_g=0.8864$ m/s, $G_s=1.5$ kg/(m$^2$s), $D_t=10.5$ m): (a) $\varepsilon_s=0.05$; (b) $\varepsilon_s=0.2$.

4 Model Evaluation

4.1 Numerical description

To further evaluate the effect of the slip velocity factor in the new drag model, we performed a series of simulations of three fluidized beds by using the EMMS/bubbling drag with and without
slip factor. These three fluidized beds operate over regimes from bubbling fluidized bed
(Dubrawski et al. [33]) to turbulent fluidized bed (Venderbosch [6], Gao et al. [36]). Fig. 3 shows
their geometries and Table 3 lists the material properties and operating conditions.

Fig. 3 Schematic diagrams of the simulated fluidized beds: (a) bubbling fluidized bed from
Dubrawski et al. [33], (b) turbulent fluidized bed from Venderbosch [6], (c) turbulent fluidized bed
from Gao et al. [36].

Table 3 Material properties and operating conditions of the selected fluidized beds

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_p$ (m)</td>
<td>$10.3 \times 10^{-5}$</td>
<td>$9.0 \times 10^{-5}$</td>
<td>$13.9 \times 10^{-5}$</td>
</tr>
<tr>
<td>$\rho_s$ (kg/m$^3$)</td>
<td>1560</td>
<td>1375</td>
<td>2400</td>
</tr>
<tr>
<td>$\rho_g$ (kg/m$^3$)</td>
<td>1.225</td>
<td>1.225</td>
<td>1.225</td>
</tr>
<tr>
<td>$\mu_g$ (Pa.s)</td>
<td>$1.8 \times 10^{-5}$</td>
<td>$1.7894 \times 10^{-5}$</td>
<td>$1.7894 \times 10^{-5}$</td>
</tr>
</tbody>
</table>
ANSYS Fluent® 15 was used as the CFD solver. For the bubbling fluidized bed, 9.51 kg particles were piled up in the bottom of bed to a height of 0.8 m at the beginning of simulation, and for the other two turbulent fluidized beds, 0.384 kg and 2.15 kg particles were piled up to the heights of 0.75 m and 0.204 m, respectively. The gas enters the bed from the bottom inlet with uniform velocity and exits from the top outlets, where atmospheric pressure was prescribed. The no-slip and the partial-slip boundary condition were prescribed for the gas phase and solid phase, respectively. The algebraic form of the granular temperature model is chosen in our simulations, since it can save computational time and has better numerical convergence. In addition, this option allows similar prediction as using the full granular energy balance model [9, 37-39]. The solids leaving the outlets were recirculated to the bottom through using user defined functions (UDF) to avoid serious solid entrainment. The averaged solid concentration in the dense bottom and solid flux at different heights were monitored to determine when the simulation reached quasi-steady state. We found those parameters converged to certain quasi-steady value after 20 seconds. Therefore, all simulations of reactors ran for 30 s and the data of the last 10 s were collected for averaging. More simulation settings are summarized in Table 4 and the drag formulations are provided in Supplementary material.

| $\xi_{ref}$ | 0.45 | 0.4 | 0.4 |
| $U_g$(m/s) | 0.4 | 0.6 | 1.25 |
| $u_t$(m/s) | 0.381 | 0.277 | 0.843 |
| $U_g/u_t$ | 1.049 | 2.166 | 1.48 |
Table 4 Simulation settings of three fluidized beds

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean grid size, Δ</td>
<td>198d_p, 162d_p, 112d_p</td>
<td>67d_p, 45d_p</td>
<td>62d_p, 51d_p, 41d_p</td>
</tr>
<tr>
<td>Solid inventory, kg</td>
<td>9.51</td>
<td>0.384</td>
<td>2.15</td>
</tr>
<tr>
<td>Initial bed height, H_0, m</td>
<td>0.8</td>
<td>0.75</td>
<td>0.204</td>
</tr>
<tr>
<td>Maximum solids fraction</td>
<td>0.55</td>
<td>0.63</td>
<td>0.63</td>
</tr>
<tr>
<td>Unsteady formulation</td>
<td>Unsteady, 2nd-order Implicit</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure-velocity coupling</td>
<td>Phase coupled SIMPLE</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Granular viscosity</td>
<td>Gidaspow</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Granular bulk viscosity</td>
<td>Lun et al.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Frictional viscosity</td>
<td>Schaeffer</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Granular temperature</td>
<td>Algebraic</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Frictional pressure</td>
<td>Based KTGF</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solid pressure</td>
<td>Lun et al.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Radial distribution</td>
<td>Lun et al.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Angle of internal friction</td>
<td>30</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Drag model</td>
<td>Hong et al. [5]/This work</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Time step</td>
<td>0.0005 s</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
bed by the axial profiles of solids volume fraction. Both drag models show good prediction and weak dependence on the grid size. Fig. 5 shows the instantaneous and time-averaged distribution of solid concentration under different resolutions when using both drag models. It is clear that meso-scale structures in forms of bubbles or voids can be captured. The predicted expansion heights, as summarized in Table 5, are determined by following the approach of Cloete et al. [40] and they are also weakly dependent on the grid size.

As shown in Fig. 5, both large and small bubbles are captured when using the finest grid resolution in the simulation. For the case of coarsest grid resolution, only large bubbles are captured. Vashisth et al. [41] also reported similar results. The probable reason is that only the bubble larger
than the grid size can be captured in CFD simulation. Although different bubble behaviors are captured by using different grid resolutions, such difference does not result in much different time-averaged distribution of solid concentration, bed expansion and axial profiles of solid concentration, suggesting that both structure-dependent drag models allow quantitative prediction under coarse grid resolution though flow details are filtered.
Fig. 5 Instantaneous and time-averaged distribution of solid concentration of the bubbling fluidized bed of Dubrawski et al. [33] by using drag models of (a) Hong et al. [5] and (b) this work.
Table 5 Expansion heights predicted for the bubbling fluidized bed under different grid sizes

<table>
<thead>
<tr>
<th>Grid size</th>
<th>Expansion height (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Hong et al. [5]</td>
</tr>
<tr>
<td>57$d_p$</td>
<td>1.155</td>
</tr>
<tr>
<td>112$d_p$</td>
<td>1.162</td>
</tr>
<tr>
<td>162$d_p$</td>
<td>1.185</td>
</tr>
<tr>
<td>198$d_p$</td>
<td>1.203</td>
</tr>
</tbody>
</table>

Fig. 6 compares the radial profiles of solid concentration when using both drag models under the coarsest resolution ($\Delta=198d_p$). It is clear that both models capture the so-called core-annulus flow structure. Quantitative comparison to experimental data shows that both drag models allow reasonable prediction and their difference is small. This finding is consistent with the report of Ghadirian et al. [42], as the bubbling fluidized bed is operated with low gas velocity and a narrow distribution of slip velocity. Therefore, it is not surprising that the slip factor is not so significant here.
Fig. 6 Comparison of time-averaged radial profiles of solid concentration at the height of (a) $H=0.24$ m, (b) $H=0.4$ m, (c) $H=0.56$ m and (d) $H=0.72$ m.

4.2.2 Turbulent fluidized bed

In the following, we present results of two turbulent fluidized beds to further investigate the effect of newly introduced slip factor on the grid dependence. Fig.7 shows time-averaged axial profiles of solid concentration and several slices of distribution of solids. Two drag models are employed under two resolutions. When the EMMS/bubbling drag of Hong et al. [5] is employed, refining grid size from $67d_p$ to $45d_p$ obviously improves the prediction, especially in the dense bottom. Whereas for the new drag model, the prediction is less sensitive to the change of grid size and the axial profiles under both grid resolutions agree well with the experiment.
Fig. 7 Time-averaged axial profiles of solid concentration and distribution of solid concentration over the whole turbulent fluidized bed of Venderbosch [6] when using (a) the drag of Hong et al. [5] and (b) this work.

Compared to the case of Venderbosch, the fluidized bed of Gao et al. [36] is operated with higher gas velocity. The simulated axial profiles of time-averaged solid concentration by using both drag models are shown in Fig.8. Three grid resolutions were employed. For the EMMS/bubbling model of Hong et al. [5], the prediction improves with grid refinement. However, the case with finest resolution (Δ=41dp) still underestimates the solid concentration in the bottom region and overestimates the solid concentration in the top of bed. When the new drag model is applied, the grid size has little effect on the predicted curves and at the same time the simulation results are much closer to the experiment, reflecting the contribution of the slip velocity.
Fig. 8 Time-averaged axial profiles of solid concentration for turbulent fluidized bed of Gao et al.\[36\] under different grid sizes by using the drag models of (a) Hong et al.\[5\] and (b) this work.

Fig. 9 shows the relative errors (R=|\(\varepsilon_s,c - \varepsilon_s,f\)|/\(\varepsilon_s,f\)×100%) of solid concentration. For the model of Hong et al.\[5\], almost all the relative errors of solid concentration in the dense bottom exceed 5% and some even larger than 10%. By comparison, the relative errors of using the new drag model are much smaller.

Fig. 9 The relative errors of solid concentration by using the model of Hong et al.\[5\] and new
drag model (relative error $R=\frac{|\epsilon_{s,c} - \epsilon_{s,f}|}{\epsilon_{s,f}} \times 100\%$, where $\epsilon_{s,c}$ is solid concentration under the coarsest grid resolution, and $\epsilon_{s,f}$ under the finest grid resolution).

Fig. 10 shows radial profiles of time-averaged solid concentration at different heights under the coarsest grid resolution ($\Delta \approx 62d_p$). At the lower positions of $H=0.078$ m and 0.138 m, the prediction of the EMMS/bubbling model of Hong et al. [5] is generally lower than that of this work in most regions, especially near the wall. At higher position of 0.338 m, the results predicted by using both drag models are close to each other. At even higher position of $H=0.478$ m, the new drag model again shows better agreement with experimental data.

Fig. 10 The radial profiles of time-averaged solid concentration for turbulent fluidized bed of Gao et al. [36] at different heights: (a) $H=0.078$ m, (b) $H=0.138$ m, (c) $H=0.338$ m and (d) $H=0.478$ m.
5 Conclusions

The EMMS/bubbling drag model is extended to the sub-grid level by following the two-step scheme of EMMS/matrix model. The heterogeneity index is therefore correlated as a function of both local voidage and slip velocity. Simulations over a periodic domain show that the new drag model is less sensitive to grid size because of the additional dependence on local slip velocity. When applying the new drag model to simulations of realistic fluidized beds, we find that such additional dependence on slip velocity enables better grid-independent results for high-velocity turbulent fluidized beds. Compared to our previous EMMS/bubbling model, the new drag model shows better qualitative agreement with experimental data.

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$</td>
<td>acceleration</td>
<td>m/s²</td>
</tr>
<tr>
<td>$C_{d0}$</td>
<td>standard drag coefficient for a particle</td>
<td></td>
</tr>
<tr>
<td>$C_{db}$</td>
<td>standard drag coefficient for a bubble</td>
<td></td>
</tr>
<tr>
<td>$C_{dc}$</td>
<td>effective drag coefficient for a particle in dense phase</td>
<td></td>
</tr>
<tr>
<td>$C_{dc0}$</td>
<td>standard drag coefficient for a particle in dense phase</td>
<td></td>
</tr>
<tr>
<td>$C_{df}$</td>
<td>effective drag coefficient for a particle in dilute phase</td>
<td></td>
</tr>
<tr>
<td>$C_{df0}$</td>
<td>standard drag coefficient for a particle in dilute phase</td>
<td></td>
</tr>
<tr>
<td>$C_{db0}$</td>
<td>effective drag coefficient for a bubble</td>
<td></td>
</tr>
<tr>
<td>$d_b$</td>
<td>bubble diameter</td>
<td>m</td>
</tr>
<tr>
<td>$d_{bm}$</td>
<td>maximum bubble diameter</td>
<td>m</td>
</tr>
<tr>
<td>$d_p$</td>
<td>particle diameter</td>
<td>m</td>
</tr>
<tr>
<td>$D_t$</td>
<td>column diameter</td>
<td>m</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td>------</td>
</tr>
<tr>
<td>$F$</td>
<td>drag force</td>
<td>N</td>
</tr>
<tr>
<td>$f$</td>
<td>volume fraction of dense phase</td>
<td></td>
</tr>
<tr>
<td>$g$</td>
<td>gravity acceleration</td>
<td>m/s$^2$</td>
</tr>
<tr>
<td>$g_0$</td>
<td>radial distribution function</td>
<td></td>
</tr>
<tr>
<td>$H$</td>
<td>fluidized bed height</td>
<td>m</td>
</tr>
<tr>
<td>$H_D$</td>
<td>heterogeneity index</td>
<td></td>
</tr>
<tr>
<td>$N_{st}$</td>
<td>mass-specific energy consumption for suspending and transporting particles</td>
<td>W/kg</td>
</tr>
<tr>
<td>$N_T$</td>
<td>total mass-specific energy</td>
<td>W/kg</td>
</tr>
<tr>
<td>$p$</td>
<td>pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number ($Re=\frac{U \rho_d \rho_g}{\mu_g}$)</td>
<td></td>
</tr>
<tr>
<td>RR</td>
<td>relative error</td>
<td>%</td>
</tr>
<tr>
<td>$u$</td>
<td>velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>$u_t$</td>
<td>terminal velocity of a single particle</td>
<td>m/s</td>
</tr>
<tr>
<td>$U_g$</td>
<td>superficial gas velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>$U_s$</td>
<td>superficial solid velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>$U_r$</td>
<td>slip velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>$U_{rc}$</td>
<td>slip velocity in dense phase</td>
<td>m/s</td>
</tr>
<tr>
<td>$U_{rt}$</td>
<td>slip velocity in dilute phase</td>
<td>m/s</td>
</tr>
<tr>
<td>$U_{ri}$</td>
<td>slip velocity in inter phase</td>
<td>m/s</td>
</tr>
</tbody>
</table>

Greek letters

1

2 Greek letters
\( \beta \) effective drag coefficient \( \text{kg/(m}^3\text{s)} \)

\( \beta_0 \) Wen & Yu drag coefficient \( \text{kg/(m}^3\text{s)} \)

\( \varepsilon \) voidage

\( \varepsilon_{\text{end}} \) minimum fluidization voidage

\( \mu \) viscosity \( \text{Pa} \cdot \text{s} \)

\( \rho \) density \( \text{kg/m}^3 \)

Subscripts

- \( b \) bubble phase
- \( c \) dense phase
- \( f \) dilute phase
- \( g \) gas
- \( gc \) dense-phase gas
- \( gf \) dilute-phase gas
- \( s \) solid phase
- \( sc \) dense-phase solid
- \( sf \) dilute-phase solid

Acknowledgments

This work is financially supported by the National Natural Science Foundation of China under Grant nos. 21576263, 21625605 and 91334204, and the “Strategic Priority Research Program” of Chinese Academy of Sciences under no. XDA07080202, and the Youth Innovation
Promotion Association CAS no.2015033.
References


