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Simon Schneiderbauer
Johannes Kepler University, Austria

Stefan Puttinger
Johannes Kepler University, Austria

Stefan Pirker
Johannes Kepler University, Austria

VERIFICATION OF SUB-GRID DRAG MODIFICATIONS FOR DENSE GAS-PARTICLE FLOWS IN BUBBLING FLUIDIZED BEDS

Simon Schneiderbauer[a]*, Stefan Puttinger[a] and Stefan Pirker[a,b]
[a]Johannes Kepler University; CD Laboratory on Particulate Flow Modelling
Altenbergerstr. 69, 4040 Linz, Austria
[b]Johannes Kepler University; Inst. of Fluid Mechanics and Heat Transfer
Altenbergerstr. 69, 4040 Linz, Austria
*T: +43-(0)-732-2468-6482; E: simon.schneiderbauer@jku.at

ABSTRACT
The application of coarse meshes enables the investigation of industrial scale reactors using kinetic theory based two-fluid models (TFM). Many sub-grid drag modifications have, therefore, been put forth by academic researchers to account for the effect of small unresolved scales on the resolved meso-scales in this case. However, all these models significantly differ in terms of their dependencies on the void fraction and on the particle slip velocity. We, therefore, thoroughly implemented the sub-grid drag models of (i) EMMS, (ii) Kuipers, (iii) Sundaresan and (iv) Simonin and compared them to (v) our CD-Lab relation and to (vi) the homogenous drag law of Wen and Yu in case of a three dimensional bubbling fluidized bed. The results are verified a fine grid reference simulation. It is shown that the latter is not able to determine the hydrodynamics of the bed properly. Even though the application of the different sub-gird drag models significantly impacts the flow of the solid, the superficial gas flow seems to be quite insensitive to the sub-grid drag model. In contrast, predictions of each drag modification of the bed expansion show fairly good agreement with the resolved results. However, it appears that the coarse grid simulations considerably overestimate the bubble rise velocity. Second, the CD-Lab modification is validated in case of a pseudo-2D bubbling fluidized bed. The numerical results obtained on a coarse gird demonstrate that the CD-Lab model reveals fairly good agreement with experimental data of bed expansion.

INTRODUCTION
Fluidized beds and moving beds are widely used in process industries, for example, for biomass reactors, polymerization reactors, metallurgical processes and for the discharge of granular materials from silos. However, due to computational limitations a fully resolved simulation of industrial scale reactors is unfeasible (1). Andrews *et al.* (2) suggested that a grid-independent solution can be obtained up to the grid size in the order of 10 particle diameters. In recent years, several approaches has been proposed to account for the effect of the small unresolved scales on the interphase momentum exchange when using two-fluid models with coarse meshes. Parmentier *et al.* (1) and Igci *et al.* (3, 4) derived residual correlations from filtering fully resolved simulations. The EMMS approach (5–7) is based on the assumption that heterogeneous structures form, which require additional modeling. The resulting underdetermined set of equations is solved by minimizing a cost function, referred to as stability condition. Wang *et al.* (8) proposed a modification of homogenous drag models to account for heterogeneous structures in bubbling fluidized beds, where the volume fraction of the bubbles is based on empirical correlations. Finally, Schneiderbauer *et al.* (9, 10) proposed a sub-grid drag modification referred to the

CD-Lab model. This approach can be regarded as considerable simplification of the EMMS model. By ignoring the drag on the particles in the dilute phase the underlying EMMS balance equations (5–7) can be solved rendering an additional stability condition unnecessary. Furthermore, in contrast to EMMS the CD-Lab model distinguishes between resolved and unresolved clusters by computing the expectation value of the diameter of the unresolved clusters. This, in turn, implies that the drag modification recovers the homogenous drag law as the solids volume fraction approaches the maximum packing of frictional spheres.

An adequate modeling of the unresolved part of the drag is essential to predict the correct bed expansion (1). In fact, the bed expansion appears to be nearly independent on the unresolved contribution of the particle stress. However, it has to be noted that although the magnitude of the drag force is much larger than the particle stresses, neglecting their unresolved contribution produces quantitative changes in the predicted results (4).

However, the general applicability of above mentioned modifications of homogenous drag correlations to bubbling fluidized beds is unverified. For example, the EMMS model was originally developed for risers. Igci *et al.* (4) accounted for frictional stresses at solids volume fractions only above 0.59 when deriving the residual correlations for the effective drag. However, frictional stresses may become important even at significantly smaller solids volume fractions (11–13). Parmentier *et al.* (1) introduced a parameter, which is dynamically adjusted by a second filter operation, to obtain best match between the coarse grid simulations and the corresponding fully resolved data.

In this paper, we present a verification study of these state-of-the-art TFM sub-grid modifications of the drag law for dense-gas particle flows. These are applied to a bubbling fluidized bed of fine glass particles. The numerical results are analyzed with respect to the bed expansion, time averaged solids volume fraction, time averaged superficial gas flow, time averaged particle mass fluxes and bubble properties including bubble size and bubble rise velocities. Furthermore, the CD-Lab model is validated by experimental data using a different stetting. Finally, a conclusion ends this paper.

TEST CASE DESCRIPTION

To study the sub-grid drag correlations in the bubbling/slugging regime we investigated a gas-solid fluidized bed of Geldart B glass particles. A simple case with a superficial vertical gas velocity $W_g^{in} = 0.21$ m s^{-1} at the inflow is studied by using the kinetic theory based TFM model for gas-particle flows of Schneiderbauer *et al.* (11, 14). At the side walls we apply a no-slip boundary condition for the gas phase and a partial slip boundary conditions for the solid phase (15). The physical parameters are given in Table 1 (11–13). The dimensions of the fluidized bed are given in Figure 1. Note for the experimental validation of the CD-Lab model the depth of the bed was 20 mm and the initial bed height $h_0 = 0.2$ m.

Following our previous studies (11, 14) we apply the CFD solver TFM equations (table 5), whereby the sub-grid drag modifications are not covered by its standard functional range. These are, therefore, implemented by user defined functions. For

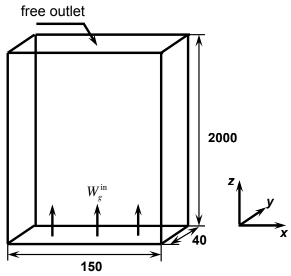

Figure 1: Sketch of the bubbling fluidized bed geometry. The dimensions are in mm.

property		value	unit
particle diameter	d_s	150	µm
particle density	ρ_s	2500	kg m^{-3}
air density	ρ_g	1.224	kg m^{-3}
solids volume fraction at maximum packing	ϵ_s^{max}	0.6	-
initial bed height	h_0	0.5	m
superficial gas velocity at minimum fluidization conditions	U_g^{mf}	0.08	m s^{-1}
terminal settling velocity	u_t	0.96	m s^{-1}

Table 1: Physical parameters

further details the reader is referred to (9).

VERIFICATION OF SUB-GRID DRAG MODIFICATIONS

We obtained a time-dependent solution using a grid spacing $\Delta_f = 8d_s$, which is assumed to be sufficiently fine to resolve all heterogeneous structures, referred to as reference solution. Thus, we used the homogenous drag correlation of Wen and Yu (16). To study the applicability of sub-grid modifications of the groups of EMMS, Kuipers, Sundaresan, Simonin and our CD-Lab relation to bubbling fluidized beds, we repeated this simulation using a grid spacing of $\Delta_c = 64d_s$ (coarse grid).

In a first step, we focus on the impact of drag modifications only in this study. Thus, we do not account for the sub-grid stress modifications proposed by Igci *et al.* (3, 4). Furthermore, we do not include the dynamic adjustment procedure of Parmentier *et al.* (1), since their result suggest that in case of 2D fluidized bed the adjustment parameter K appears nearly independent of the vertical coordinate and is approximately 4. We, therefore, study the applicability of this simplification using an unadjusted ($K = 1$) and an adjusted case with constant $K = 4$.

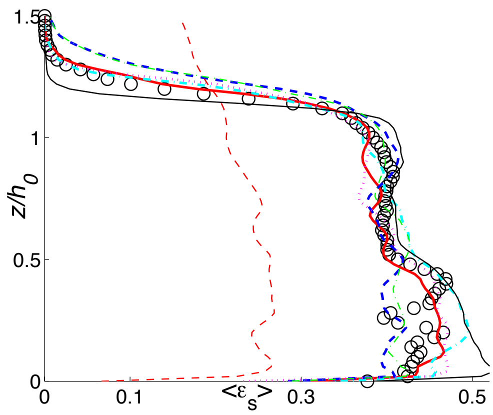

Figure 2: Axial profiles of the time averaged solids volume fraction, ϵ_s, for superficial gas velocity $W_g^{in} = 0.21$ m s^{-1} and a grid spacing of 64 particle diameters: --- β of CD-Lab (*9*, *10*); – · – β of Parmentier *et al.* (*1*) with $K = 4$; – – – β of Parmentier *et al.* (*1*) with $K = 1$; · · · β of Wang *et al.* (*8*); --- EMMS (*5*–*7*); – · – β of Igci *et al.* (*3*, *4*); – – – β of Wen and Yu (*16*); o fine grid simulation.

Particle Volume Fraction

In Figure 2 a comparison of the time-averaged axial profile of the solids volume fraction ϵ_s is shown. Firstly, it is observed that neglecting sub-grid inhomogeneities, i.e. using the drag law of Wen and Yu, leads to a significant overprediction of the bed expansion using the coarse grid. In fact, the bed expansion is overestimated considerably (by about 80%) compared to the fully resolved reference simulation. This, in turn, implies that using the homogenous drag correlation on coarse grids underestimates the time averaged volume fractions within the bed.

Second, we investigated the behavior of the fluidized bed when applying the different sub- grid drag closures on the coarse grid ($\Delta_c = 64d_s$). Remarkably, although these reveal significant different dependencies on the slip velocity and the solids volume fraction Figure 2 clearly demonstrates that the predicted bed expansions are in fairly good agreement with the resolved data.

Bubble size and rise velocity

Additionally, we may ask whether the coarse grid simulations are able to predict the mean bubble diameters and the bubble rise velocity sufficiently. Thus, we evaluate the bubble properties via digital image analysis of the volume fraction maps of the center plane. The methodology follows the procedure presented by Li *et al*. (17). In a first step, the solid fractions are exported to a linear gray scale map and then converted to binary images by applying a constant grey scale threshold of 0.6. After thresholding all self-contained areas are detected as bubbles, where valid area-centroids are limited to values between $0.05h_0$ and h_0. This procedure eliminates on the one hand, all small bubbles close to the distributor plate, which tend to merge very quickly. On the other hand, all erupting bubbles are excluded as soon as they have an open connection to the void section above the bed. In a second processing step, the identified bubbles are matched between two consecutive time steps in the sense of a Lagrangian object tracking.

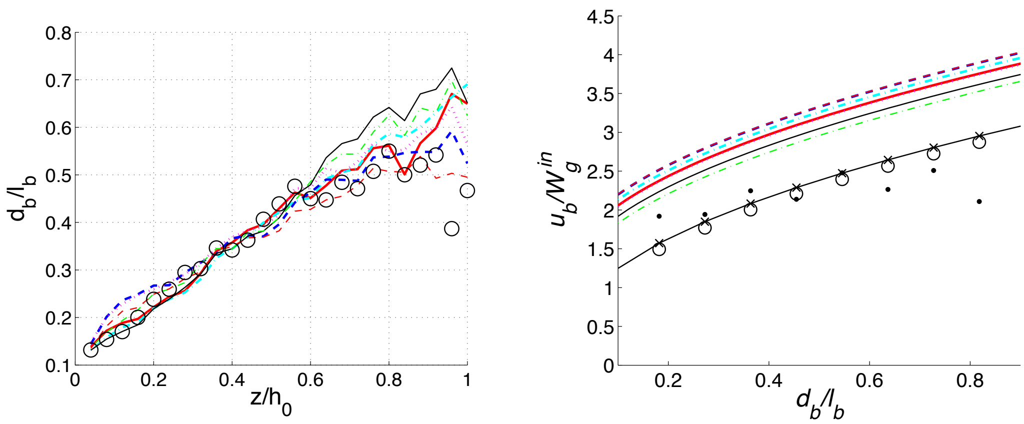

Figure 3: a) Dimensionless mean bubble diameter as a function of the normalized height z/h_0 and b) dimensionless bubble rise velocity u_b/W_g^{in} as a function of the normalized bubble diameter d_b/l_b for $W_g^{in} = 0.21$ m s^{-1} and a grid spacing of 64 particle diameters. l_b denotes the width of the bed. The points indicate the raw data of the bubble rise velocity obtained from the fine grid simulation. -X- experimental correlation (18). Note that β_{WY} is nearly indistinguishable from $\beta_P^{(K=1)}$. The lines and symbols have the same meaning as in Figure 2.

In Figure 3a the corresponding dimensionless mean bubble diameter as a function of the normalized height z/h_0 is plotted. Remarkably, each drag modification is in fairly good agreement with the bubble size obtained from the resolved simulation for $z/h_0 < 0.8$, that is the increasing bubble diameter with decreasing hydrostatic pressure. It is interesting to note that even the homogenous drag correlation of Wen and Yu yields the bubble diameter appropriately. Above $z/h_0 = 0.8$ the resolved simulation additionally reveals small bubbles indicated by the decreasing mean bubble diameter with height. Such small bubbles are not observed on the coarse grid since their size is of Δ_c.

The bubble rise velocity u_b in a freely bubbling fluidized bed is usually correlated to the bubble diameter by (18)

$$u_b = \psi\left(W_g^{in} - U_g^{mf}\right) + C\sqrt{g d_b},$$

where $C \approx 0.5$ (19). To compare the different sub-grid drag modifications with the resolved data we regress the visual flow rate ψ from the computed bubble rise velocities. Figure 3b reveals that each coarse grid simulation considerably overestimates the rise velocity of the bubbles compared to the experimental correlation (18) and the fine grid simulation although the size of the bubbles is consistent with the resolved simulation. The raw data (not shown here) suggests that primarily the rise velocity of the larger bubbles is substantially overpredicted by the coarse grid simulations. This, in turn, implies that the countercurrently downflowing layer of particles around these larger bubbles is not resolved adequately supporting the demand of sub-grid stress closures.

Superficial Gas Flow and Particle Mass Flux

Figure 4a compares the axial profiles of the time averaged dimensionless superficial gas velocities. The figure shows that the coarse grid superficial gas velocities are in good agreement with the fine grid simulation for all drag modifications in case of $z/h_0 < 1$. The application of the homogenous drag correlation of Wen and Yu, however, fails to predict the gas flow in the fluidized bed.

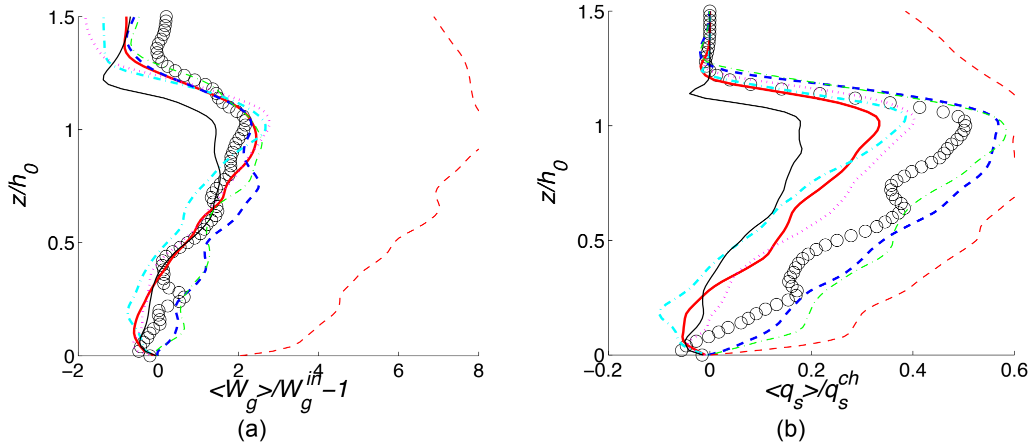

Figure 4: Axial profiles of a) the time averaged dimensionless superficial gas velocity in verticaldirection, $\langle W_g \rangle / W_g^{in} - 1$, and b) of the time averaged dimensionless particle mass flux in vertical direction, $\langle q_s \rangle / q_s^{ch}$ ($q_s^{ch} = \epsilon_s^{max} \rho_s u_t$), for $W_g^{in} = 0.21$ m s^{-1} and a grid spacing of 64 particle diameters. The lines and symbols have the same meaning as in Figure 2.

Figure 4a shows the variations of the corresponding dimensionless solids mass flux, which is made dimensionless using a characteristic solid flux, $q_s^{ch} = \epsilon_s^{max} \rho_s u_t$. Similar to the resolved case, the coarse grid simulations yield rising particles in the center of the bed and slowly downward flowing particles in the dense side region. (not shown here). However, the particle phase mass flux is on the one hand, underestimated by the adjusted Simonin, the EMMS, the Kuipers and the CD-Lab drag and on the other hand, marginally overestimated by the remaining sub-grid drag modifications.

VALIDATION OF CD-LAB SUB-GRID DRAG MODIFICATION

We investigated the fluidized bed shown in Figure 1 with a depth of 20 mm and a initial bed height $h_0 = 0.2$ m experimentally. The behavior of the particles in the vicinity of the front plane has been recorded using a high speed cam (Fastcam SA3 Model 120k). By averaging the resulting gray-scale images the time averaged solids volume fraction can be deduced locally (Figure 5). Note at the bottom of the fluidized bed the area below $z = 10$ mm was not accessible with the camera.

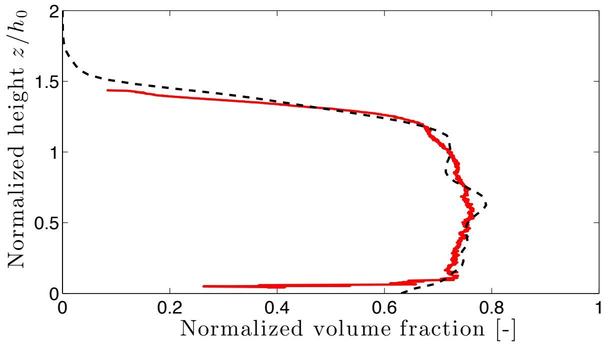

Figure 5: Axial profiles of the time averaged solids volume fraction, ϵ_s, for superficial gas velocity $W_g^{in} = 0.21$ m s^{-1} and a grid spacing of 64 particle diameters: – – – β of CD-Lab (*10*); ––– experiment

We obtained a time-dependent coarse grid solution using a grid spacing of $\Delta_c = 64 d_s$. In Figure 5 a comparison of the time-averaged axial profiles of the solids volume fraction, ϵ_s, for $W_g^{in} = 0.21$ m s^{-1} is shown. It is observed that using the CD-Lab drag modification yields a fairly good estimation of the bed expansion and the computed volume fraction profile highly correlates with the experimental data.

NOTATION

β	drag coefficient	Δ	grid spacing
ε_s	volume fraction of solid phase	d_b	bubble diameter
g	standard acceleration due to earths gravity	q_s	particle mass flux
u_t	terminal settling velocity of an isolated particle	u_b	bubble rise velocity
W_g	superficial gas velocity		

Note the remaining symbols are defined in Table 1.

CONCLUSIONS AND OUTLOOK

We have presented a verification study of the state-of-the-art sub-grid drag modifications of the groups of EMMS (5–7), Kuipers (8), Sundaresan (3, 4), Simonin (1) and the CD-Lab model (10) in case of a bubbling fluidized bed. A sub-grid drag correlation accounts for unresolved sub-grid structures in contrast to homogeneous drag laws. The results are discussed with respect to fully resolved reference simulations. Note that we did not include any sub-grid modification for the unresolved part of the particle stresses to investigate the impact of the drag closures independently. This study reveals that:

- Applying a homogenous drag law, which ignores unresolved sub-grid structures, fails to predict the hydrodynamics of the bubbling fluidized bed using a coarse realistic meshes.
- Applying each of the discussed sub-grid drag modifications reveals the bed expansion adequately.
- The bubble size is estimated suitably by the investigated sub-grid drag closures.
- However, the bubble rise velocity is significantly overestimated by these closures, which indicates the requirement of sub-grid stress modifications for the frictional regime.
- The model Parmentier *et al.* (1) predicts the main features of the bubbling fluidized bed correctly even for a constant adjustment parameter, that is $K = 4$.
- Compared to the resolved simulation the computational demand is reduced by approximately two orders of magnitude using the coarse grid for equal time step sizes. Coarse meshes, however, allow larger time steps that additionally improves the computational efficiency by approximately one order of magnitude in our study.
- The CD-Lab model shows fairly good agreement with measurements of the bed expansion.

To conclude, this study demonstrates that the discussed sub-grid drag modifications are applicable to bubbling fluidized beds. However, several tasks remain. First, it is necessary to study the impact of the unresolved part of the particle stresses (4) on the hydrodynamics of a bubbling fluidized bed. These may have a considerable impact on the computed bubble rise velocities. Second, the impact of the dynamic adjustment procedure of Parmentier et al. (1) should be studied for more general fluidized beds. Third, the models should be investigated with respect to the bubble shape, i.e. weather the models reveal sharp distinct or smooth blurred bubbles. Finally, the models must be further validated by experimental data. This will be discussed in future publications.

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