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Quantitative Assessment of Fine-Grid Kinetic-Theory-Based Predictions of Mean-Slip in Unbounded Fluidization

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Significance

The quantitative ability of a kinetic-theory-based, two-fluid model is demonstrated in a clustering (unstable) gas-solid system via highly resolved simulations. Unlike previous works, this assessment is validated against ideal computational fluid dynamics-discrete element method data to minimize sources of discrepancy. Overall, good agreement in mean-slip velocities is observed with relative errors less than 20% over a mean solids concentration range of 0.02–0.25. Local concentration gradient distributions are also studied, showing a distinct shift toward higher gradients at higher mean solids concentrations which is proposed as the bottleneck in obtaining grid-independence rather than the cluster length scale. *AIChE J*, 62: 11–17, 2016

Keywords: clustering instability, fluidization, sedimentation, computational fluid dynamics, two-fluid model

Introduction

Understanding and accurately predicting the dynamic behavior of gas-solid flows are important for the chemical and energy process industries, among others, that utilize bubbling and circulating fluidized beds (BFBs/CFBs). Unfortunately, the two-phase behavior in such devices is incredibly complex. One of the most challenging aspects of accurately modeling gas-fluidized particulates is the clustering instability, which is a persistent, transient, inhomogeneous spatial distribution of solids concentration, as exemplified in Figure 1. Such heterogeneous structures have a large impact on mass, momentum, and energy transport, thus playing an important role in the design and scale up of industrial devices.

For several decades, since the pioneering work of Tsuo and Gidaspow,[2] it has been known that continuum two-fluid models (TFM) are able to *qualitatively* capture such dynamic inhomogeneities. Figure 1 demonstrates such qualitative agreement comparing a snapshot from a discrete-particle simulation in which particle dynamics are solved explicitly (on the left, results of Radl and Sundaresan[1]), with a similar snapshot from a continuum simulation in which particle dynamics are modeled (on the right, current results). However, to accurately simulate such complex dynamics, numerical grids capable of resolving all relevant scales are required, as shown by Agrawal et al.[3] In dilute clustered flows, grids as small as 10 particle diameters are required for numerical accuracy. The scale-resolution requirement is even more demanding in dense regions, such as in a bubbling bed, where grid sizes approaching the particle diameter become necessary.[4] With typical particle sizes on the order of 10^{-5} to 10^{-3} m and typical system sizes on the 10^{-1} to 10^{1} m, it is easy to see that full-scale resolution of industrial and even pilot-scale devices is impractical, particularly in three-dimensions (3-D).

Due to this impractical computational overhead, strategies to model, rather than directly simulate, the small-scale clustering dynamics remains an active area of research. Several methods have been explored such as the Energy Minimization Multiscale method,[5–7] structure-dependent drag laws,[8–11] and the filtered TFM approach.[12–15] Filtered TFMs do not directly resolve all length scales of the particle clusters so that coarse grids can be utilized, but additional closure modeling is required to account the effects of clustering at scales smaller than the filter. Filtered models rely on fully resolved simulations to constitute subgrid closures, most of which utilize TFMs derived from kinetic theory (KT). However, as pointed out by Zhou et al.,[11] the ability of fine-grid continuum simulations to accurately reproduce dynamic clustering behavior without introducing a modified drag correlation remains an open question. This concern was also recognized by Igci

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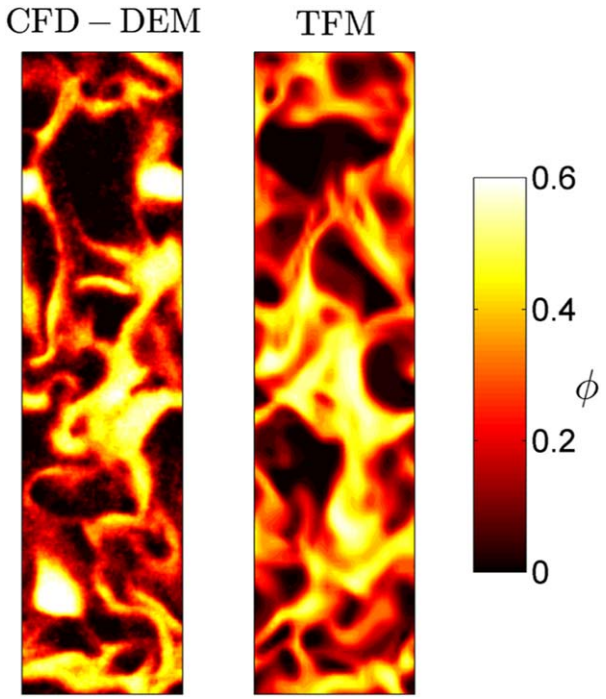

Figure 1. Comparison of instantaneous clustering dynamics between CFD-DEM (left) and a KT-based TFM (right) in the *xy*-plane at a mean solids concentration of $\langle\phi\rangle=0.25$.

CFD-DEM data provided by Stefan Radl, for more details on CFD-DEM methodology, see Radl and Sundaresan.[1] [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

et al.[12] Nevertheless, most subsequent efforts have focused on verifying that fine-grid simulations are accurately reproduced by filtered models on coarse grids[16–18] and validating the coarse-grid filtered model,[19–22] rather than validating the underlying KT-based TFM itself, which has several inherent assumptions and approximations of its own.

Although quantifying the accuracy of KT-based TFMs to predict clustered gas-solid flows has received limited attention, several previous contributions have been made. Wang[23] used fine-grid simulation to capture clustering in a small region of an experimental CFB riser and compared the root mean square (RMS) fluctuation in concentration as a function of averaged concentration. He was able to show good quantitative agreement with the measured data by comparing least-squares best-fit curves of the RMS. Benyahia[24] simulated a larger (10-m tall) CFB and compared the vertical void fraction profile to one deduced from pressure profile measurements. Cloete et al.[25] presented a similar analysis to Benyahia[24] that included chemical reactions and also compared radial solids concentration and velocity profiles. However, Cloete et al.[25] recognized that complete grid-independence was probably not achieved.

Despite these prior quantitative assessments of clustering predictions using highly resolved TFMs, several aspects of the comparisons hamper a straightforward interpretation of the results. First, all three studies highlighted above[23–25] involved a dimensional mismatch in which two-dimensional (2-D) simulations were compared with 3-D data. It has become increasingly clear that significant quantitative differences exist between 2-D and 3-D simulations.[22,26] Second, all of the quantitative assessments referenced above have been validated with experimental data. While the ultimate goal is to use such modeling tools for the design and scale up of real-world devices, experimental data is often not a "clean" test of KT-based TFMs, as noted by Wang et al.[4] Real particles are neither perfectly spherical nor monodisperse, which is assumed in the KT derivation. Additionally, other physically relevant phenomena that are neglected in the KT-based TFM (e.g., gas-phase turbulence, humidity, van der Waals forces, electrostatics, etc.) are often present in existing experimental data and can only be effectively eliminated with carefully controlled experiments (see, for example, LaMarche et al., submitted). To overcome such challenges, "ideal" numerical data provided by discrete-particle simulations is a logical first step in the TFM validation process. For example, CFD-DEM, which utilizes computational fluid dynamics (CFD) to resolve the fluid phase and discrete element method (DEM) to track individual particles, is an attractive option for generating numerical data and was used by Wang et al.[4] validating a KT-based TFM for the "inverse" instability, that is, bubbles in dense bed. CFD-DEM does not resolve all scales of the fluid flow like direct numerical simulation (DNS)-DEM, but this allows the same drag law to be applied to both CFD-DEM and TFM, further isolating the validation of the continuum closures – solids pressure, solids viscosity, and so forth – for use in clustering systems. Other pseudodiscrete-particle methods, such as multiphase particle-in-cell (MP-PIC), do not present such ideal validation data as MP-PIC also relies on (empirical) continuum closures.[27,28]

In this work, the recent high-resolution CFD-DEM simulations by Radl and Sundaresan[1] of an unbounded, 3-D fluidization (or sedimentation) system are used as ideal data to validate clustering predictions of a KT-based TFM[29] solved on a fine numerical grid. The global Favre-averaged, mean-slip velocity is used as the test variable. Overall, the comparisons are quite good, providing evidence that fine-grid continuum simulations accurately capture dynamic clustering behavior using a traditional (locally homogeneous) drag law. In addition to the fine-grid simulations, systematic grid coarsening was also used to study the convergence behavior in an effort to resolve some apparent confusion of resolution requirements that appears in the literature.[25,30,31] Similar to previous studies, we find that solution independence is a function of mean solids concentration. However, it is proposed that the concentration gradient at the cluster interface is responsible for controlling the convergence behavior, rather than oft-cited cluster length scale (see, for example[3,32–34]).

Two-Fluid Model Description

The continuum model used in the following analysis is the recently developed KT-based TFM of Garzó, Tenneti, Subramaniam, and Hrenya[29] (GTSH). The GTSH theory decomposes the effects of the interstitial fluid into three contributions: mean drag, which is associated with the mean particle velocity; thermal drag, which corresponds to the fluctuating (peculiar) particle velocity; and the neighbor effect, a stochastic source of fluctuating particle velocity due to the fluctuations of nearby particles transmitted through the interstitial fluid. Unlike previous KT-based TFMs, GTSH

incorporates all three components into the starting Enskog kinetic equation, which is then used to rigorously derive the continuum model. As part of the derivation, several standard simplifying assumptions were used. A few of particular interest here are: (1) the particles are smooth, frictionless, and monodisperse spheres; (2) particle collisions are instantaneous, binary and characterized by a constant coefficient of restitution; and (3) the Knudsen numbers of the continuum variables are small, (i.e., the theory is of Navier–Stokes-order).

For the sake of brevity, the GTSH model is not repeated here and the interested reader is referred to the original publication[29] for complete details. However, a few deviations from the published theory have been used which should be mentioned. While the original GTSH publication did not specify a particular drag law, the model of Beetstra et al.[35] was used here for consistency with the CFD-DEM simulations. The thermal drag and neighbor effect models of Koch and Sangani[36] are used throughout the entire concentration range, rather than a step change to the analytical models of Koch[37] at $\phi = 0.1$. Additionally, the first-order thermal-Reynolds number correction of Wylie et al.[38] is included in the thermal drag model. Finally, the radial distribution function of Carnahan and Starling[39] was replaced with that of Ma and Ahmadi,[40] which better approximates the random-close packed limit.

The open-source CFD code MFiX (https://mfix.netl.doe.gov/) is used for numerical solution of the governing equations. Developed at the National Energy Technology Laboratory, MFiX uses a finite volume discretization on a staggered grid. Time advancement is a variable time-step, semi-implicit method based on the SIMPLE family of algorithms. The Superbee flux-limiter is used for all variable extrapolation. In a comprehensive assessment of more than 20 approximately second-order upwind convection schemes, Waterson and Deconinck[41] found that the Superbee scheme performed the best for discontinuous data, as present at the interface between clustered and dilute regions. A similar result was also reported by Guenther and Syamlal[42] studying bubbles in a dense bed.

Simulation Parameters

The simulation domain is the same as that of Radl and Sundaresan.[1] The system size is $L_x = L_z = 0.8$ cm in the transverse directions and $L_y = 3.2$ cm in the vertical (streamwise) direction. A uniform discretization is used for all simulations with a grid size of $\Delta = 250$ μm. When nondimensionalized by the particle diameter, the grid size is approximately three particle diameters, that is, $\Delta^* = 3.\bar{3}$. In the transverse directions, purely periodic boundary conditions are applied with no external forces. Gravity acts in the negative vertical direction, that is, $g_y = -|\mathbf{g}| = 9.81$ m/s^2. The body force is balanced by a periodic, pressure-drop boundary condition; that is, the fluid phase pressure gradient has been decomposed into mean linear and local components, so that no net force acts on the mixture. As there are no walls, the system may be considered in a state of unbounded (infinite) fluidization or sedimentation. In the continuum simulations, the net vertical flux is set to zero, more reminiscent of sedimentation, but the distinction is meaningless in the absence of walls. (Transformations are necessary to compare phasic variables in different reference frames, but slip (relative) velocity between the phases is Galilean invariant in the current system).

The particle and fluid properties are the same as those used by Radl and Sundaresan[1]: $d_p = 75$ μm, $\rho_s = 1500$ kg/m^3, $\rho_f = 1.3$ kg/m^3, and $\mu_f = 1.8 \cdot 10^{-5}$ Pa s. The dimensionless variables characterizing the state of the system are the Archimedes number, $Ar = \rho_f \Delta\rho |\mathbf{g}| d_p^3 / \mu_f^2$, the mean solids concentration, $\langle\phi\rangle$, the density ratio, $\rho^* = \rho_s / \rho_f$, and the restitution coefficient, e, where the angle brackets indicate domain-averaged quantities. In this study, the mean solids concentration is varied and the remaining parameters are fixed at $Ar = 24.87$, $\rho^* = 1153.85$, and $e = 0.9$. Time is nondimensionalized by the single-particle characteristic time, $\tau = u_t / |\mathbf{g}|$, where $u_t = 23.2$ cm/s is the terminal velocity of a single particle in an infinite medium. Here, u_t has been obtained from the drag law of Beetstra et al.[35] in the limit of infinite dilution. One noteworthy omission from this list is the sliding particle-particle friction coefficient. Interparticle friction was considered in the original CFD-DEM simulations ($\mu_{pp} = 0.1$), although it has been neglected in the continuum model initially. The ramifications of this assumption are considered in more detail in the following section.

Initially, both phases are at rest and the granular temperature of the solid phase, a measure of fluctuating kinetic energy, is negligibly small. The solids concentration is randomly perturbed in each cell from a uniform distribution of $\pm 50\%$ about the mean value. Renormalization is applied so that the mean concentration is unchanged. This perturbation acts as an initial "kick" and helps minimize the time to reach the statistical steady state.

Results and Discussion

To assess the ability of the KT-based, GTSH continuum model to accurately predict strongly heterogeneous, dynamic clusters, we compare the mean-slip velocity to CFD-DEM results in the same unbounded fluidization domain. It is well known that clustering leads to a reduction in mean drag force compared with a homogeneous state.[3,5,8–11,43,44] The drag force within the clusters themselves is significantly higher due to the increased particle concentration. As the clusters present a large flow resistance, the gas tends to simply bypass or flow around them. The preferential gas flow in the dilute, low-resistance regions causes the increase in mean-slip.

Here, we define the slip velocity as the absolute difference in the global, Favre-averaged, streamwise phasic velocities, that is, $v_{\text{slip}} = |\langle\langle v_s \rangle\rangle - \langle\langle v_f \rangle\rangle|$, where $v_{j=s,f}$ is the local vertical component of the phasic velocities and double brackets indicate Favre averaging, for example, $\langle\langle v_s \rangle\rangle = \langle \phi v_s \rangle / \langle \phi \rangle$. In the CFD-DEM case, the solids velocity is a particle average rather than a Favre-average. Even when globally averaged, the slip velocity is still time-dependent and can vary quite significantly depending on the instantaneous structure of the system. Therefore, once a stationary state is reached, the slip velocity is then time averaged and nondimensionalized into Reynolds number form, that is, $Re_{\text{slip}} = \rho_f \bar{v}_{\text{slip}} d_p / \mu_f$, where the overbar indicates time averaging. The CFD-DEM data was time averaged for at least a $\delta t^* = 30$ nondimensional time window[1] and all TFM results have been averaged over a time window of $\delta t^* = 63.4$.

The mean and standard deviations of the time averages are reported in Figure 2 and compared with the published CFD-DEM results of Radl and Sundaresan.[1] Also shown for comparison is the homogeneous (stable), analytical solution

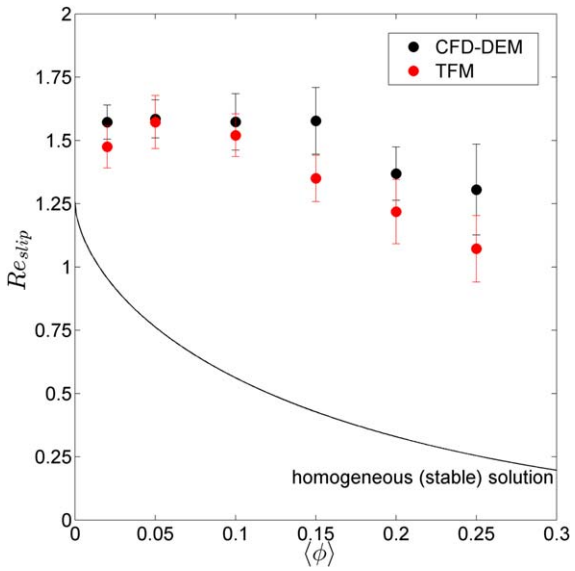

Figure 2. Comparison of mean-slip Reynolds numbers between CFD-DEM and the TFM simulations for various mean solids concentrations.

Error bars represent the standard deviation of the time averaging. The homogeneous (stable) solution is also shown for comparison. CFD-DEM data reported previously by Radl and Sundaresan,[1] and the TFM simulations are based on GTSH theory.[29] [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

obtained from the TFM (i.e., assuming all variables are constant and uniform). The qualitative agreement of the TFM simulations and CFD-DEM is excellent. The mean-slip Reynolds number of both is relatively constant and greater than the homogeneous solution (and the terminal velocity) at low solids concentration. At intermediate concentrations, the slip velocity predicted by the TFM and CFD-DEM simulations begins to decay, although remaining significantly higher than the homogeneous solution. Quantitatively, the TFM and CFD-DEM comparisons are also quite good. The TFM seems to systematically under-predict the slip velocity compared with the CFD-DEM, particularly at intermediate concentrations. However, the standard deviations overlap in all but one case and the relative error of the mean values is less than 15% in all but one case. The relative error for the six cases (low to high concentration) are: 6.2, 0.8, 3.4, 14.4, 10.9, and 17.9%. It is also important to emphasize that the drag law[35] was developed from fixed-bed DNS simulations where the (random) particle placements are globally homogeneous. More specifically, the mean drag utilized in the TFM depends only on local properties and the clustered (dynamic and heterogeneous) solution itself is responsible for increasing the mean-slip Reynolds number from the homogeneous (stable) solution. In other words, a structure-dependent drag law does not appear to be needed for fine-grid KT-based TFM simulations.

Figure 2 indicates that despite the overlapping error bars, the simulations of intermediate concentration, $\langle\phi\rangle \geq 0.15$, have a slightly higher relative error than the three more dilute cases, $\langle\phi\rangle \leq 0.10$. This demarcation coincides with the point at which clusters begin to reach the maximum packing limit, potentially straining the assumption that interparticle friction can be neglected. In the TFM data presented in Figure 2, only the plastic pressure component of the frictional stress model of Syamlal and coworkers[45,46] has been applied to restrict the solids concentration at the random-close packed limit, $\phi_{max}=0.64356$.[40] (In other words, frictional viscosity is neglected by assuming the angle of internal friction is zero). Frictional stresses were initially neglected because (1) particle friction was not incorporated into the KT derivation of the GTSH TFM; (2) most continuum frictional stress models are largely empirical[47]; and (3) mapping of DEM frictional parameters to continuum models is ambiguous. Nonetheless, in an effort to gauge the role of friction as a potential source of the mild TFM vs. CFD-DEM discrepancy at higher particle loadings, the simulations with the two highest mean concentrations were repeated using the frictional stress model of Srivastava and Sundaresan[48] using the Savage modification[45,46] implemented in MFiX. The adjustable frictional parameters are set to the suggested values[48] typically used to represent glass beads,[47] which we view as a conservative test of the significance of frictional stress in this system. The results are reported in Table 1 and compared with the frictionless TFM and (frictional) CFD-DEM results. In both cases, the inclusion of a frictional stress model increases the mean-slip Reynolds number. While this does reduce the relative error to 6.8 and 15.5% (compared with 10.9 and 17.9%. without friction, respectively), the difference remains within the standard deviation of the frictionless results and continues to under-predict the CFD-DEM data. While this limited analysis does not prove that friction is irrelevant in general, it does indicate that continuum frictional stress models play a relatively minor role in the system considered here, even for dense clusters.

In addition to the fine-grid TFM simulations, we have also performed a convergence analysis to study the effect of mean solids concentration on the resolution requirement. The numerical grid was successively coarsened, uniformly in each direction, using discretizations of $\Delta^*=4.\bar{4}$, $6.\bar{6}$, $8.\bar{8}$, and $13.\bar{3}$. For the two most dilute cases, the mean-slip Reynolds number changed very little for all grids studied, consistent with the results of Agrawal et al.[3] Conversely, as the mean concentration increases above $\langle\phi\rangle=0.05$, the required grid resolution for convergence increases. At the highest mean concentration studied here, $\langle\phi\rangle=0.25$, the finest grid resolution is required, $\Delta^*=3.\bar{3}$. Such a fine discretization is more reminiscent of dense BFBs, for example, Wang et al.[4] recommend $\Delta^* \approx 2$–4. Resolutions typical of fine-grid BFB simulations at such high mean concentrations is not surprising, given that it is difficult to distinguish qualitatively which feature is the dominant discrete constituent, that is, clusters or bubbles.

Previously, the cluster length scale has been cited as the criteria controlling the resolution requirement (see, for example[3,32–34]). However, Figure 3 illustrates that the characteristic

Table 1. Effect of Frictional Stress Modeling on Mean-Slip Reynolds Numbers for the Two Highest Mean Solids Concentrations Studied Here

	TFM	TFM with Friction	CFD-DEM
$\langle\phi\rangle=0.20$	1.219 ± 0.127	1.275 ± 0.123	1.369 ± 0.105
$\langle\phi\rangle=0.25$	1.072 ± 0.132	1.103 ± 0.103	1.306 ± 0.180

CFD-DEM data reported previously by Radl and Sundaresan.[1]

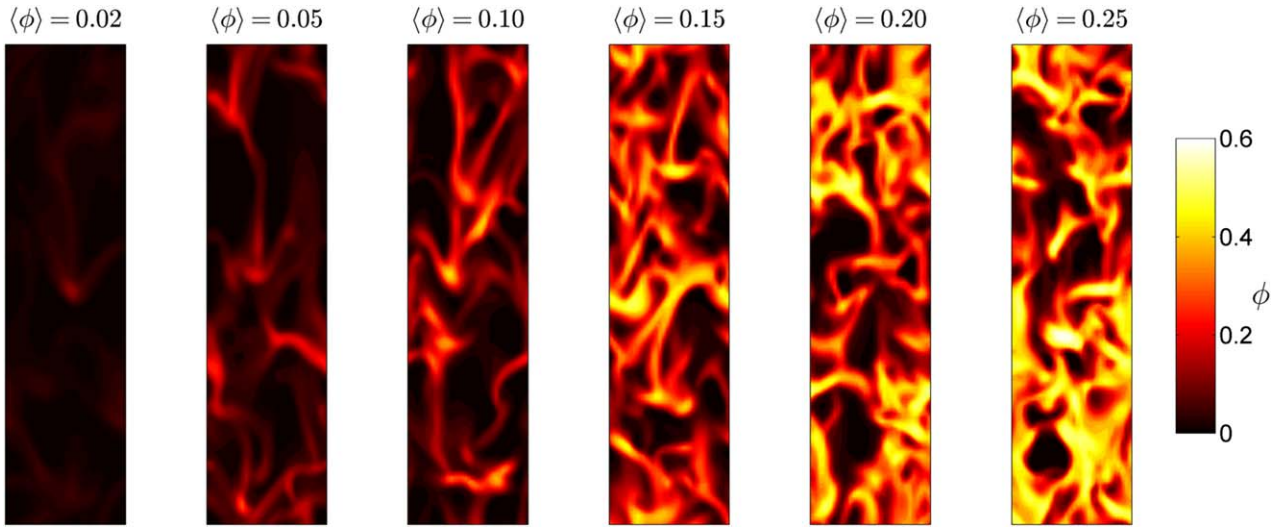

Figure 3. Instantaneous clustering patterns in the *xy*-plane for various mean solids concentrations obtained from TFM simulations.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

size of the clusters is relatively similar for all mean concentrations studied here. Accordingly, it does not appear that the cluster length scale is controlling the grid resolution required for numerical accuracy. From a discretization point of view, the most challenging aspect of these heterogeneous structures is the concentration gradient at the boundaries of the clusters. In all cases, the dilute regions have near-zero solids concentration while the cluster concentration increases with increasing mean concentration, which in turn increases the concentration gradients and thus the grid resolution requirement. To quantify this assertion, the cumulative distribution function (CDF) of the magnitude of the local concentration gradient (nondimensionalized by the particle diameter) is computed throughout the domain from 15 instantaneous samples. The results, reported in Figure 4, clearly show that the CDF of concentration gradients shift to larger values as the mean concentration increases. At $\langle\phi\rangle$=0.25, the largest nondimensional gradient approaches 0.1, which, for reference, would cause an increase in concentration from zero to maximum packing in just 6.5 particle diameters. The dependence of the local concentration gradient on the mean concentration explains why previous studies of more realistic systems, that is, domains that contain both dense and dilute regions, have found different grid resolution requirements for clustering flows.[24,25,30,31] Figure 4 also indicates that the shift of the CDFs to higher gradients is "slowing" as the mean concentration approaches conditions more typical of bubbling than clustering. Finally, it should be emphasized that these findings also strongly depend on the numerical method. Knowing that such sharp gradients must be resolved for fine-grid simulations of moderately dense clustered flows, schemes with higher resolution of discontinuous data are recommended, such as Superbee and SMART[41]; first-order schemes should be used with caution or avoided altogether.[42]

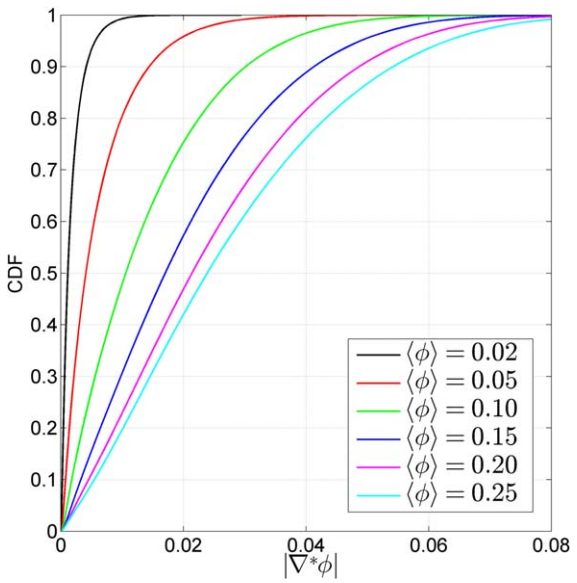

Figure 4. Cumulative distribution function of the dimensionless magnitude of the local concentration gradient obtained from 15 instances in the time-averaging window of the TFM simulations.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Conclusions and Outlook

An unbounded fluidization (or sedimentation) system has been simulated on a fine-grid in 3-D with a two-fluid model (TFM) for gas-solids flow. The continuum model used here is the recently developed, KT-based theory of Garzó et al.,[29] which incorporates mean drag, thermal drag, and a neighbor effect into the starting Enskog kinetic equation. The results have been quantitatively compared with the high-resolution CFD-DEM numerical data of Radl and Sundaresan.[1]

The domain- and time-averaged mean-slip velocity is used to test the ability of continuum simulations to predict the

CFD-DEM data, with excellent agreement over the entire range of concentrations. Qualitatively, both TFM and CFD-DEM simulations lie well above the analytical homogeneous (stable) solution due to clustering, which creates a reduced effective drag due to flow bypass. Quantitatively, the TFM-DEM agreement is also quite good, with relative errors less than 10% for dilute concentrations of $\langle\phi\rangle \leq 0.10$ and 10–20% at intermediate concentrations of $\langle\phi\rangle \geq 0.15$. The incorporation of friction into the TFM slightly decreases the error, although the results indicate that even dense clusters are relatively insensitive to friction. It should be pointed out, although, that this analysis does not absolve all of the assumptions violated by the TFM when very dense clusters are present; specifically, the assumption of binary, nonenduring contacts is inherent to KT and distinct from the assumption of smooth, frictionless spheres.

Additionally, the discretization requirement for fine-grid (i.e., fully resolved or grid-independent) solutions is investigated. Consistent with previous reports, dilute clustering flows ($\langle\phi\rangle \sim 0.05$) may reach convergence with a relatively modest grid of 10–20 particle diameters[3]; this cutoff gradually decreases with increasing concentration until grids of two to four particle diameters[4] are required at moderate-to-dense mean concentrations ($\langle\phi\rangle \sim 0.25$). Our results suggest that the concentration gradient is responsible for this increase in grid resolution, rather than the commonly cited cluster length scale, (see, for example[3,32–34]). This hypothesis is supported by comparing the CDFs of the nondimensional concentration gradient, which increase consistently with increasing mean concentration whereas the cluster length scale remains relatively constant.

The aforementioned increase in gradients at the dense/dilute interface of the clusters gives rise to another question, namely whether the assumption of low Knudsen numbers (i.e., small gradients), which corresponds to a truncation of the Chapman–Enskog expansions to Navier–Stokes-order in the KT derivation, is being violated. A related analysis of a granular (no fluid) homogeneous cooling system indicates that strict adherence to this assumption does not appear necessary,[49] similar to the Navier–Stokes equations for single-phase flows working well outside of their intended range of validity. However, additional mechanisms for clustering are present in two-phase gas-solid systems, and further investigation on this issue is required.

By comparing to ideal CFD-DEM data and matching system dimensions (i.e., 3-D), this work presents clean evidence that clustering characteristics can be accurately captured with a KT-based TFM solved on a fine grid. However, it should be noted that the analysis is an indirect clustering assessment as the comparison relied on the mean-slip velocity, a global- and time-averaged quantity. Qualitative agreement of dynamic structures coupled with the quantitative agreement of mean flow properties *implies* that dynamic properties are also being accurately captured. However, more thorough analyses aimed at quantifying local and/or dynamic cluster properties remains as future work.

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Literature Cited

1. Radl S, Sundaresan S. A drag model for filtered Euler-Lagrange simulations of clustered gas-particle suspensions. *Chem Eng Sci*. 2014;117:416–425.
2. Tsuo YP, Gidaspow D. Computation of flow patterns in circulating fluidized-beds. *AIChE J*. 1990;36(6):885–896.
3. Agrawal K, Loezos PN, Syamlal M, Sundaresan S. The role of meso-scale structures in rapid gas–solid flows. *J Fluid Mech*. 2001;445:151–185.
4. Wang JW, van der Hoef MA, Kuipers JAM. Why the two-fluid model fails to predict the bed expansion characteristics of Geldart A particles in gas-fluidized beds: a tentative answer. *Chem Eng Sci*. 2009;64(3):622–625.
5. Li J, Kwauk M. *Particle-Fluid Two-Phase Flow: The Energy-Minimization Multi-Scale Method*. Beijing: Metallurgical Industry Press, 1994.
6. Yang N, Wang W, Ge W, Li JH. CFD simulation of concurrent-up gas-solid flow in circulating fluidized beds with structure-dependent drag coefficient. *Chem Eng J*. 2003;96(1–3):71–80.
7. Wang W, Li JH. Simulation of gas-solid two-phase flow by a multi-scale CFD approach—extension of the EMMS model to the sub-grid level. *Chem Eng Sci*. 2007;62(1–2):208–231.
8. Beetstra R, van der Hoef MA, Kuipers JAM. A lattice-Boltzmann simulation study of the drag coefficient of clusters of spheres. *Comput Fluids*. 2006;35(8–9):966–970.
9. Wang SA, Lu HL, Liu GD, Sheng ZH, Xu PF, Gidaspow D. Modeling of cluster structure-dependent drag with Eulerian approach for circulating fluidized beds. *Powder Technol*. 2011;208(1):98–110.
10. Shah MT, Utikar RP, Tade MO, Evans GM, Pareek VK. Effect of a cluster on gas-solid drag from lattice Boltzmann simulations. *Chem Eng Sci*. 2013;102:365–372.
11. Zhou GF, Xiong QG, Wang LM, Wang XW, Ren XX, Ge W. Structure-dependent drag in gas-solid flows studied with direct numerical simulation. *Chem Eng Sci*. 2014;116:9–22.
12. Igci Y, Andrews AT, Sundaresan S, Pannala S, O'Brien T. Filtered two-fluid models for fluidized gas-particle suspensions. *AIChE J*. 2008;54(6):1431–1448.
13. Wang JW, van der Hoef MA, Kuipers JAM. Coarse grid simulation of bed expansion characteristics of industrial-scale gas-solid bubbling fluidized beds. *Chem Eng Sci*. 2010;65(6):2125–2131.
14. Parmentier JF, Simonin O, Delsart O. A functional subgrid drift velocity model for filtered drag prediction in dense fluidized bed. *AIChE J*. 2012;58(4):1084–1098.
15. Schneiderbauer S, Pirker S. Filtered and heterogeneity-based subgrid modifications for gas-solid drag and solid stresses in bubbling fluidized beds. *AIChE J*. 2014;60(3):839–854.

16. Igci Y, Sundaresan S. Verification of filtered two-fluid models for gas-particle flows in risers. *AIChE J*. 2011; 57(10):2691–2707.
17. Schneiderbauer S, Puttinger S, Pirker S. Comparative analysis of subgrid drag modifications for dense gas-particle flows in bubbling fluidized beds. *AIChE J*. 2013; 59(11):4077–4099.
18. Sarkar A, Sun X, Sundaresan S. Verification of sub-grid filtered drag models for gas-particle fluidized beds with immersed cylinder arrays. *Chem Eng Sci*. 2014;114:144–154.
19. Jiradilok V, Gidaspow D, Damronglerd S, Koves WJ, Mostofi R. Kinetic theory based CFD simulation of turbulent fluidization of FCC particles in a riser. *Chem Eng Sci*. 2006;61(17):5544–5559.
20. Benyahia S. On the effect of subgrid drag closures. *Ind Eng Chem Res*. 2010;49(11):5122–5131.
21. Igci Y, Pannala S, Benyahia S, Sundaresan S. Validation studies on filtered model equations for gas-particle flows in risers. *Ind Eng Chem Res*. 2012;51(4):2094–2103.
22. Li TW, Pannala S, Shahnam M. CFD simulations of circulating fluidized bed risers, part II: evaluation of differences between 2D and 3D simulations. *Powder Technol*. 2014;254:115–124.
23. Wang JW. High-resolution Eulerian simulation of RMS of solid volume fraction fluctuation and particle clustering characteristics in a CFB riser. *Chem Eng Sci*. 2008; 63(13):3341–3347.
24. Benyahia S. Fine-grid simulations of gas-solids flow in a circulating fluidized bed. *AIChE J*. 2012;58(11):3589–3592.
25. Cloete S, Johansen ST, Amini S. An assessment of the ability of computational fluid dynamic models to predict reactive gas-solid flows in a fluidized bed. *Powder Technol*. 2012;215-216:15–25.
26. Xie N, Battaglia F, Pannala S. Effects of using two- versus three-dimensional computational modeling of fluidized beds - Part I, hydrodynamics. *Powder Technol*. 2008;182(1):1–13.
27. Benyahia S, Galvin JE. Estimation of numerical errors related to some basic assumptions in discrete particle methods. *Ind Eng Chem Res*. 2010;49(21):10588–10605.
28. Benyahia S, Sundaresan S. Do we need sub-grid scale corrections for both continuum and discrete gas-particle flow models? *Powder Technol*. 2012;220:2–6.
29. Garzó V, Tenneti S, Subramaniam S, Hrenya CM. Enskog kinetic theory for monodisperse gas–solid flows. *J Fluid Mech*. 2012;712:129–168.
30. Lu BN, Wang W, Li JH. Searching for a mesh-independent sub-grid model for CFD simulation of gas-solid riser flows. *Chem Eng Sci*. 2009;64(15):3437–3447.
31. Li TW, Gel A, Pannala S, Shahnam M, Syamlal M. CFD simulations of circulating fluidized bed risers, part I: grid study. *Powder Technol*. 2014;254:170–180.
32. Andrews AT, Loezos PN, Sundaresan S. Coarse-grid simulation of gas-particle flows in vertical risers. *Ind Eng Chem Res*. 2005;44(16):6022–6037.
33. De Wilde J. Reformulating and quantifying the generalized added mass in filtered gas-solid flow models. *Phys Fluids*. 2005;17(11):113304-1–113304-14.
34. Wang JW. A review of Eulerian simulation of Geldart A particles in gas-fluidized beds. *Ind Eng Chem Res*. 2009; 48(12):5567–5577.
35. Beetstra R, van der Hoef MA, Kuipers JAM. Drag force of intermediate Reynolds number flow past mono- and bidisperse arrays of spheres. *AIChE J*. 2007;53(2):489–501.
36. Koch DL, Sangani AS. Particle pressure and marginal stability limits for a homogeneous monodiperse gas-fluidized bed: kinetic theory and numerical simulations. *J Fluid Mech*. 1999;400(1):229–263.
37. Koch DL. Kinetic-theory for a monodisperse gas-solid suspension. *Phys Fluids A - Fluid Dyn*. 1990;2(10): 1711–1723.
38. Wylie JJ, Koch DL, Ladd AJ. Rheology of suspensions with high particle inertia and moderate fluid inertia. *J Fluid Mech*. 2003;480:95–118.
39. Carnahan NF, Starling KE. Equation of state for nonattracting rigid spheres. *J Chem Phys*. 1969;51(2):635–636.
40. Ma D, Ahmadi G. A kinetic-model for rapid granular flows of nearly elastic particles including interstitial fluid effects. *Powder Technol*. 1988;56(3):191–207.
41. Waterson NP, Deconinck H. Design principles for bounded higher-order convection schemes—a unified approach. *J Comput Phys*. 2007;224(1):182–207.
42. Guenther C, Syamlal M. The effect of numerical diffusion on simulation of isolated bubbles in a gas-solid fluidized bed. *Powder Technol*. 2001;116(2–3):142–154.
43. Li JH, Kwauk M. Multiscale nature of complex fluid-particle systems. *Ind Eng Chem Res*. 2001;40(20):4227–4237.
44. Heynderickx GJ, Das AK, De Wilde J, Marin GB. Effect of clustering on gas-solid drag in dilute two-phase flow. *Ind Eng Chem Res*. 2004;43(16):4635–4646.
45. Syamlal M, Rogers W, O'Brien TJ. *MFIX Documentation: Theory Guide*. Energy USDo; Morgantown, WV: Morgantown Energy Technology Center; 1993. DOE/METC-94/1004 (DE94000087). Available at: https://mfix.netl.doe.gov/documentation/Theory.pdf.
46. Benyahia S. Validation study of two continuum granular frictional flow theories. *Ind Eng Chem Res*. 2008;47(22): 8926–8932.
47. Johnson PC, Nott P, Jackson R. Frictional collisional equations of motion for particulate flows and their application to chutes. *J Fluid Mech*. 1990;210:501–535.
48. Srivastava A, Sundaresan S. Analysis of a fractional-kinetic model for gas-particle flow. *Powder Technol*. 2003;129(1–3):72–85.
49. Mitrano PP, Zenk JR, Benyahia S, Galvin JE, Dahl SR, Hrenya CM. Kinetic-theory predictions of clustering instabilities in granular flows: beyond the small-Knudsen-number regime. *J Fluid Mech*. 2014;738:R2-1–R2-12.

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