Particle mixing rates using the two-fluid model

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ABSTRACT

In this work, a new methodology is introduced to calculate the solids mixing rate in dense gas-fluidized beds using the two-fluid model. The implementation of this methodology into an existing two-fluid model code was carefully verified. The solids phase continuity equation was satisfied using our method, and the sensitivity of the computational results to the time step, computational cell size, and discretization scheme was investigated to determine the optimal simulation settings. Using these simulation settings, the degree of solids mixing was observed to rapidly (exponentially) increase with increasing operating pressure and linearly decrease with increasing bed diameter. Our novel methodology can be applied to analyze mixing processes in large lab-scale beds as an alternative to existing time-consuming simulation techniques such as computational fluid dynamics combined with the discrete element model.

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Introduction

Computer simulations have become increasingly popular in the last decade in various scientific fields such as fluidization. Several mathematical models have been developed in the fluidization field including the direct numerical simulation method (Moin & Mahesh, 1998), computational fluid dynamics with discrete element model (CFD–DEM) (Tsuji, Kawaguchi, & Tanaka, 1993), the two-fluid model (TFM) (Ding & Gidaspow, 1990), the direct simulation Monte Carlo method (Tsuji, Tanaka, & Yonemura, 1998), and the discrete bubble model (Bokkers, Laverman, van Sint Annaland, & Kuipers, 2006). These models are based on certain simplifying assumptions that are often necessary to simulate the behavior of complex systems such as gas–solid fluidized beds. A robust model with less simplifications generally leads to more detailed information than a model with more assumptions. However, simplified models enable the simulation of large-scale beds within an acceptable amount of computational time.

CFD–DEM is a Eulerian–Lagrangian approach that considers the gas phase as a continuous phase where every particle is tracked individually. Because all the forces exerted on particles, including the contact forces, must be calculated for every time step, it is only possible to simulate relatively small lab-scale fluidized beds using this model. Thus, the simulation of fluidized beds containing more than 1 million particles with CFD–DEM is extremely time-consuming using standard computational resources. Conversely, the TFM is a Eulerian–Eulerian approach that considers both the gas and solids phase as continuous interpenetrating phases. The TFM uses more assumptions to represent the particulate phase motion than CFD–DEM. Therefore, it is possible to simulate large, lab-scale fluidized beds with the TFM much faster than with CFD–DEM. However, the continuum assumption for the solids phase makes it impossible to track the motion of individual particles to study, for instance, solids mixing. Therefore, it is not possible to obtain particle-scale solids information using TFM simulations, and the simulation of mixing using the TFM is not as straightforward as with CFD–DEM.

The determination of particulate phase mixing rates is critical for processes that are prone to the formation of local extreme inhomogeneities such as those encountered in gas-phase polymerization processes. Polymerization reactions are extremely exothermic, and if the particles do not mix well, the undesirable formation of hotspots (and consequently agglomerates) may occur (Godlieb, 2010). The mixing rate of granular materials is also critical in blending sensitive products such as pharmaceutical powders. Various studies (Huilin & Gidaspow, 2003; Huilin, Yurong, &

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Nomenclature

AR	Aspect ratio
CFP	Continuity fulfillment parameter
d, D	Diameter (m)
e	Particle–particle restitution coefficient
e_w	Particle–wall restitution coefficient
g_0	Radial distribution function
g	Gravitational acceleration (m/s^2)
H	Height (m)
L	Length (m)
MI	Mixing index
MW	Molecular weight (g/mol)
N_T	Number of tracers
n_r	Number of cells in the radial direction
n_θ	Number of cells in the azimuthal direction
n_z	Number of cells in the axial direction
p_c	Critical state pressure (Pa)
P	Pressure (Pa)
q_s	Pseudo-Fourier fluctuating kinetic energy flux (kg/s^3)
SI	Separation index
t	Time (s)
u	Velocity (m/s)
V	Volume (m^3)
X	Position vector, fraction of colored particles
Z	Height (m)

Greek letters

β	Interphase momentum transfer coefficient (kg/(m^3 s))
γ	Dissipation of granular energy due to inelastic particle–particle collisions (kg/(m s^3)), normalized solids content
Δr	Computational grid size in the radial direction (m)
Δt	Computational time step (s)
Δz	Computational grid size in the axial direction (m)
$\Delta \theta$	Computational grid size in the azimuthal direction
ε	Volume fraction
κ_s	Pseudo thermal conductivity (kg/(m s))
λ_s	Solid bulk viscosity (Pa s)
ρ	Density (kg/m^3)
τ	Newtonian stress tensor (Pa)
θ	Granular temperature (m^2/s^2)
μ_s	Shear viscosity (Pa s)
μ_s^f	Frictional stress tensor (Pa s)
φ	Angle of internal friction (°)

Subscripts and superscripts

0	Initial
f	Frictional
g	Gas
N	Normalized
r	Radial direction
s	Solid
sim.	Simulation
z	Axial direction

Greek subscripts

θ	Azimuthal direction

Abbreviations

CFD	Computational fluid dynamics
DEM	Discrete element model
FOU	First-order upwind
KTGF	Kinetic theory of granular flow
TFM	Two-fluid model

Table 1
Mathematical representation of TFM based on the KTGF.

$$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\right) + \nabla\cdot\left(\varepsilon_g\rho_g\vec{u}_g\right) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\right) + \nabla\cdot\left(\varepsilon_s\rho_s\vec{u}_s\right) = 0 \tag{2}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_g\vec{u}_g\right) + \nabla\cdot\left(\varepsilon_g\rho_g\vec{u}_g\vec{u}_g\right) = \tag{3}$$
$$-\varepsilon_g\nabla P_g - \nabla\cdot\left(\varepsilon_g\bar{\bar{\tau}}_g\right) - \beta\left(\vec{u}_g - \vec{u}_s\right) + \varepsilon_g\rho_g\vec{g}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\vec{u}_s\right) + \nabla\cdot\left(\varepsilon_s\rho_s\vec{u}_s\vec{u}_s\right) = \tag{5}$$
$$-\varepsilon_s\nabla P_g - \nabla P_s - \nabla\cdot\left(\varepsilon_s\bar{\bar{\tau}}_s\right) + \beta\left(\vec{u}_g - \vec{u}_s\right) + \varepsilon_s\rho_s\vec{g}$$

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\varepsilon_s\rho_s\theta\right) + \nabla\cdot\left(\varepsilon_s\rho_s\theta\vec{u}_s\right)\right] = -\left(P_s\bar{\bar{I}} + \varepsilon_s\bar{\bar{\tau}}_s\right): \tag{6}$$
$$\nabla\vec{u}_s - \nabla\cdot\left(\varepsilon_s q_s\right) - 3\beta\theta - \gamma$$

Gidaspow, 2003; van Sint Annaland et al., 2009a, 2009b; Wang et al., 2014) have used the TFM with the help of the multi-fluid model based on the kinetic theory of granular flow to determine the solids mixing rate when there is more than one solid phase in the bed, each with different physical properties. However, there is not much research on the determination of the solids mixing rate when all the particles have the same physical properties. Deen, Willem, Sander, and Kuipers (2010) attempted to overcome this disadvantage of TFM and determine the solids mixing rate for fluidized beds with one particle type using tracers representing the solids phase motion. Implementation of this technique in an existing TFM code (Verma, Deen, Padding, & Kuipers, 2013) revealed that this technique suffers from certain deficits in accurately predicting the solids motion. In the present work, the accuracy of this technique will be assessed, and a new method for the characterization of solids mixing using the TFM will be introduced. After implementation and verification of this new method in an existing in-house TFM code, the sensitivity of the computational results with respect to the grid size, time step, and discretization scheme will be investigated. Finally, the effects of pressure and bed size on the solids mixing in a fluidized bed will be studied in detail.

Governing equations

Table 1 presents the TFM governing equations based on the kinetic theory of granular flow (KTGF). Eqs. (1) and (2) present the continuity (mass conservation) equations for the gas and solids phases, respectively. Eqs. (3) and (4) are the Navier–Stokes equations (momentum conservation equations) for the gas and solids phases, respectively, and Eq. (5) presents the governing equation for the solids phase granular temperature. The summation of the gas and solid volume fraction is equal to one for every computational cell. The implementation of these equations for 3D cylindrical systems and experimental validation were presented by Verma et al. (2013). The same in-house code was used in this work. In addition to the main governing equations, closure equations are required, which follow Nieuwland, van Sint Annaland, Kuipers, and van Swaaij (1996) in Table 2.