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Original Research Paper

Tracking of particles using TFM in gas-solid fluidized beds

M. Banaei [a,b,*], J. Jegers [a], M. van Sint Annaland [a,b], J.A.M. Kuipers [a,b], N.G. Deen [b,c]

[a] Multiphase Reactors Group, Department of Chemical Engineering & Chemistry Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands
[b] Dutch Polymer Institute (DPI), P.O. Box 902, 5600 AX Eindhoven, The Netherlands
[c] Multiphase and Reactive Flows Group, Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

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ABSTRACT

In this work, a new method is presented to track discrete tracer particles in a two fluid model (TFM). This method is particularly useful for studying features of discrete particles, such as solids mixing. Following the implementation and verification of this method, its accuracy was studied. The results showed that the new method fulfills the continuity equation and it can represent individual solids motion very well. This method may suffer from false diffusion, which can be diminished by selecting a sufficiently small grid size. In addition, it has several advantages over other techniques, like simplicity, ease of implementation, straightforward processing and enabling the calculation of a mixing index based on the initial neighbor distance concept. Moreover, this method can open a new way to combine the TFM with Lagrangian approaches. After analyzing the strengths and drawbacks of our method and finding the proper simulation settings, the effects of superficial gas velocity and restitution coefficient on solids mixing were investigated. The results showed that the solids mixing is enhanced by increasing the gas velocity and/or decreasing the restitution coefficient. The observed trends can be attributed to altered bubble formation and dynamics. These results also confirm our earlier findings on the solids temperature distribution in fluidized beds for polyolefins production (Banaei et al., 2017).

1. Introduction

Gas-solid fluidized beds have been used in various physical and chemical processes for several decades. Due to their importance and their wide range of applications, numerous experimental and simulation techniques have been introduced to understand the behavior of these contactors. Simulation techniques have become increasingly interesting to researchers because of the enormous improvements in the performance of computer processors during the last several years. As a consequence, several mathematical models have been presented and examined for the prediction of fluidized bed reactors. These models can even give some detailed information about the fluidized bed features that are not easily accessible through experiments. The two fluid model (TFM) based on the kinetic theory of granular flow (KTGF) is one of these models that has been used for the prediction of the behavior of fluidized beds.

The TFM is an Eulerian-Eulerian model and considers the gas and the solids phase(s) as continuum phases. In other words, the continuity equation and the volume-averaged Navier-Stokes equations are used in this model to describe the gas and solids motion. This model has been validated and used by many researchers in the field of fluidization and it has shown its strength in different aspects [2–5]. However, this model has some drawbacks as well. For example, it is not feasible to track individual particles with this model. As a result, it is not straightforward to calculate the solids mixing patterns with the TFM. In one of our earlier works, a new method for overcoming this difficulty was introduced and the deficiencies of other approaches were investigated [6]. In the earlier proposed approach, the solids phase was divided into several colored groups and the motion of each group was obtained by solving the scalar convection equations. Even though the solids mixing rate and the solids mixing pattern can be obtained by this technique, it is not possible to track individual particles. In this work, another methodology for the calculation of the solids mixing is introduced. The main advantage of this method is that individual particles can be tracked, which opens a new window for combining the TFM with Lagrangian approaches. In addition, the new method makes quantification of the solids mixing much more straightforward. For example, there is no need to perform two different sets

* Corresponding author at: Multiphase Reactors Group, Department of Chemical Engineering & Chemistry Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands.
E-mail address: mohammad.banaei@outlook.com (M. Banaei).

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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 (–)
f_i	solids flow at the cell face *i* (kg/s)
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 in the whole bed (–)
Nr	number of cells in the radial direction (–)
n_t	number of tracers in one cell (–)
Nθ	number of cells in the azimuthal direction (–)
Nz	number of cells in the axial direction (–)
P	pressure (Pa), probability (–)
q_s	pseudo-Fourier fluctuating kinetic energy flux (kg/s^3)
r_{ij}	distance between tracer *i* and tracer *j* (m)
T	time (s), mixing time (s)
U	velocity (m/s)
V	volume (m^3), velocity (m/s)
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^3 s)), 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 (–)
Δ	a parameter that shows the direction of solids flow at cell faces (–)
Ε	volume fraction (–)
κ_s	pseudo thermal conductivity (kg/(m s))
λ_s	solid bulk viscosity (Pa s)
Ρ	density (kg/m^3)
Τ	stress tensor (Pa/m)
Θ	granular temperature (m^2/s^2)
Μ	viscosity (Pa s)

Subscripts and superscripts

0	initial
F	frictional
G	gas
L	leaving
Nl	not leaving
R	radial direction
S	solid
sim.	simulation
Z	axial direction

Greek subscripts

Θ	azimuthal direction

Abbreviations

CFD	computational fluid dynamics
DEM	discrete element model
FRB	freeboard
KTGF	kinetic theory of granular flow
TFM	two fluid model

of simulations or solve mixing equations twice with different initial settings to obtain the solids mixing rate in the horizontal and vertical directions.

This method has a high level of accuracy and it can be implemented very easily because of its simple concept, as will be explained in detail later. In this sections, the new method will be demonstrated to study the solids mixing in poly-olefin fluidized beds. In earlier work, it is showed that the solids mixing rate has a profound effect on the probability of hot-spot formation [1]. For this reason, the results of this work complement our earlier research. Additionally, the new method can also be used to investigate the solids mixing in other applications, especially when other techniques like the discrete element model (DEM) would require too much computational time.

This paper is organized as follows. After the description, implementation and verification of the method, the fulfillment of the solids phase continuity equation by this technique is checked. Subsequently, the sensitivity of the model results with respect to the time step and computational cell size is examined. Moreover, also deficiencies of this technique are investigated. Finally, the effect of the superficial gas velocity and restitution coefficient on the mixing rate of particles is explored and the results are analyzed and discussed thoroughly.

2. Governing equations

The mathematical representation of the TFM governing equations are given in Table 1 where Eqs. (1) and (2) present the mass conservation or continuity equations for the gas and solids phases respectively. Eqs. (3) and (4) are the volume-averaged Navier-Stokes equations for both phases. Eq. (5) is the granular temperature equation that describes the kinetic energy associated with the solids phase fluctuating motion.

The governing equations are closed with closures that were previously presented by Nieuwland et al. [7] and are given in Table 2.

Details about the implementation and verification of these equations was presented by Verma et al. [12]. The finite difference technique was used to solve the TFM equations. The interested reader is referred to the aforementioned work for further details about the applied numerical algorithms and verification steps.

3. Tracking of particles

The method for tracking individual particles consists of several steps and it starts with the initialization of tracers in the bed based on the solids content in every computational cell. After solving the

Table 1
TFM governing equations in vector form based on the KTGF.

$\frac{\partial}{\partial t}(\varepsilon_g\rho_g) + \cdot(\varepsilon_g\rho_g\vec{u}_g) = 0$	(1)
$\frac{\partial}{\partial t}(\varepsilon_s\rho_s) + \cdot(\varepsilon_s\rho_s\vec{u}_s) = 0$	(2)
$\frac{\partial}{\partial t}(\varepsilon_g\rho_g\vec{u}_g) + \cdot(\varepsilon_g\rho_g\vec{u}_g\vec{u}_g) = -\varepsilon_g P_g - \cdot(\varepsilon_g\vec{\vec{\tau}}_g) - \beta(\vec{u}_g - \vec{u}_s) + \varepsilon_g\rho_g\vec{g}$	(3)
$\frac{\partial}{\partial t}(\varepsilon_s\rho_s\vec{u}_s) + \cdot(\varepsilon_s\rho_s\vec{u}_s\vec{u}_s) = -\varepsilon_s P_g - P_s - \cdot(\varepsilon_s\vec{\vec{\tau}}_s) + \beta(\vec{u}_g - \vec{u}_s) + \varepsilon_s\rho_s\vec{g}$	(4)
$\frac{3}{2}[\frac{\partial}{\partial t}(\varepsilon_s\rho_s\theta) + \cdot(\varepsilon_s\rho_s\theta\vec{u}_s)] = -(P_s\vec{\vec{I}} + \varepsilon_s\vec{\vec{\tau}}_s) : \vec{u}_s - \cdot(\varepsilon_s q_s) - 3\beta\theta - \gamma$	(5)