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Stochastic bubble developing model combined with Markov process of particles for bubbling fluidized beds

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HIGHLIGHTS

- The calculation speed of stochastic model is 70 times faster than CFD–DEM.
- A spherical cap bubble model is established.
- The development of bubbles is simulated in stochastic model.
- The disturbance of bubbles to the particles is concerned.
- The pulsating characteristics of particle mixing is improved a lot.

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ABSTRACT

This paper describes a new stochastic model for simulating particle movement in bubbling fluidized beds (BFB). The model includes a stochastic bubble developing model (SBDM) and a Markov chain based stochastic model (MCM) of particles, while current single MCM for BFB cannot afford detailed flow structure of gas and solid for further chemical reaction modeling. The bubble generating, moving and growing sub-models of SBDM are detailed introduced. SBDM is coupled with MCM by a bubble shaping sub-model. Stochastic methods and some empirical models are used in the modeling process. Samples used by the stochastic model are taken from a CFD–DEM result. Four representative cases that have different fluidized air velocities are simulated. Particle distribution and mixing calculated by CFD–DEM, MCM and SBDM–MCM are compared. Results show both MCM and SBDM–MCM can approximately reduce the computing time by 70 times compared with CFD–DEM, and they can also keep the macroscopic characteristic of particle movement well from CFD–DEM. But MCM always shows a time-averaged result, and it cannot present the structure and disturbance of bubbles. While SBDM–MCM successfully simulates the development of bubbles and introduces their instantaneous disturbance to the movement of particles. Compared with MCM, the remarkable improvement of SBDM–MCM is that it can give the recurrence of bubble structure in particle distribution and the pulsating characteristics of particle mixing curves.

1. Introduction

Fluidized beds are widely applied in practical engineering, including in the chemical and energy industry, which commonly involve interaction, reaction, mass transfer and heat transfer between fluid gas and bed material. Modeling of such processes is beneficial to understand, design and optimize the entire process. Traditional empirical and semi-empirical models (such as plug flow model [1] and bubbling two-phase model [2]) have high efficiency and quick response, but they cannot provide detailed movement of particles and bubbles. In addition, the accuracy is not high enough. However, popular numerical approaches based on CFD have the ability to predict the actual flow as well as the thermal and concentration field [3]. Especially the Euler–Lagrangian method takes the interaction between gas phase and single particle into consideration. Furthermore, CFD–DEM contains the interaction between particles [4–6], which can more accurately simulate the gas–solid flow. But the long computing time and the high computation load are always the bottlenecks of this kind of method for practical application.

Stochastic modeling is a potential method to simulate the processes involving particles both quickly and accurately. Markov chain-based stochastic model (MCM) particularly has the advantages of simple theory, easy program and fast calculation. MCM

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Nomenclature

d_t	equivalent-area circle diameter of a bubble at time t
D_I	distance from a particle in region I to C_1 before bubble coupling
D'_I	distance from a particle in region I to C_1 after bubble coupling
D_{II}	distance from a particle in region II to C_1 before bubble coupling
D'_{II}	distance from a particle in region II to C_1 after bubble coupling
D_{III}	distance from a particle in region III to C_2 before bubble coupling
D'_{III}	distance from a particle in region III to C_2 after bubble coupling
h_t	height of a bubble centroid at time t
P	Markovian transition matrix
r_t	radius of a bubble at time t
$\mathbf{S}(t)$	state vector
Δt	transition time step (s)
u_t	rise velocity of a bubble centroid at time t
w_t	radial coordinate of a bubble centroid at time t

has been successfully applied in many granule systems, such as grinding, classification and mixing [7–13]. The statistical sampling for the calculation of transition probability matrix is one of the most important parts in the process of building MCM. Sampling by experiment is very reliable, but it needs very heavy workload to obtain enough samples. Sampling by empirical calculation is much easier, but the data that can be obtained is limited. Taking some mature CFD results as samples is the optimized choice, especially the CFD–DEM results [14–16]. Detailed and abundant particle information can be obtained by CFD–DEM, and the fundamental physics and hydromechanics based algorithm provides nice sampling credibility.

When it comes to fluidized beds, there are some clear differences compared to other granular systems (such as rotating drums and static mixers). As the interaction between solid phase and gas phase and the instantaneous disturbance caused by bubbles are very strong, existing researches [17–20] on MCM applied to fluidized beds are mostly confined to the simulation of macroscopic characteristics of particle movement, such as residence time distribution, probability distribution and concentration distribution. Besides, sampling methods are limited to the empirical calculation and a bit of experimental data aimed at only particle phase. These kinds of modeling methods can meet the most requirement of research on rotating drums and static mixers, but they cannot give a detailed recurrence of the gas–solid structure and track specific particles in fluidized beds to satisfy the further chemical reaction, mass transfer and heat transfer modeling.

In this paper, a new stochastic model sampling from CFD–DEM results is developed to simulate the particle movement in a 2D fluidized bed. The model includes a stochastic bubble developing model (SBDM) and the MCM of particles, which aims to give a recurrence of the bubble structure and take the effect of bubbles on particle movement into consideration.

2. Model description

2.1. Discrete element method

The 2D fluidized bed modeled in this paper is a batch system with no feed or withdrawal of particles. The chamber has the height of 1.05 m and the width of 0.27 m. Other parameters are listed in Table 1. At the gas inlet the uniform gas velocity is specified, and at the outlet the gas pressure-outlet boundary condition is adopted. At the walls, the no-slip wall condition for gas phase is assumed.

In this work, it is proposed to build the stochastic model sampling from the first few iterations of a CFD–DEM simulation. In CFD–DEM model, the flow of the gas phase is calculated by local averaged Navier–Stokes equations while the movement of each particle is calculated by Newton's second law. The DEM model contains the basic drag model [21] and liner spring-dashpot model [22]. The CFD–DEM approach has been used and validated in various studies of particulate systems, and the model used in the present work follows the one proposed in Ref. [23]. Necessary information of the CFD–DEM model is given in Tables 1 and 2. The CFD–DEM considers all the particle collisions in the simulation system. To speed up the search for particle collision, the DEM cell list and neighbor search technique are employed.

The actual time of CFD–DEM simulation is from 0 to 20 s, and the microscopic data obtained from 10 to 15 s, which is considered to be fully developed, is used to construct the MCM of particles and the SBDM to furtherly predict the subsequent particle movement. DEM results from 15 to 20 s are compared to the results of stochastic model in the same time period.

2.2. Markov process of particles

A Markov process can be used to model a random system that changes states according to a transition rule, and it has been widely applied to many granule systems. The definition and detailed description can be found in Ref. [24]. The three important parameters that constitute the MCM of particles are a state vector $\mathbf{S}(t)$, a transition matrix $\mathbf{P}$, and a transition time step Δt. The only way to obtain detailed particle trajectories by MCM is to discretize the BFB into physical cells. The 2D BFB is discretized to m equal divisions in width, and n equal divisions in height. One state of a particle is represented by the cell in which the particle is located. All particles cell information at a certain time t_c forms a state vector $\mathbf{S}(t_c)$ of the whole system, which is shown as

$$\mathbf{S}(t_c) = [s_1(t_c), s_2(t_c), \ldots, s_{nm}(t_c)] \quad (1)$$

Table 1
Simulation conditions and parameters of the BFB and CFD–DEM model.

Bed size	$0.27 \times 1.05 \times 0.001$ m^3
Particle density	2600 kg/m^3
Particle diameter	0.001 m
Particle number	81,000
Inlet air velocity	1.5 m/s, 1.8 m/s, 2.1 m/s, 2.4 m/s
Minimum fluidization velocity	0.44 m/s
CFD cells number	27×105
DEM cells number	90×350
CFD time step	5×10^{-5} s
DEM time step	5×10^{-6} s
Particle normal stiffness	10,000 N/m
Particle tangential stiffness	2857 N/m
Particle normal restitution coefficient	0.97
Particle tangential restitution coefficient	0.33
Particle frictional coefficient	0.1