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

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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 modelling 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

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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.

Keywords: Stochastic model; Markov chain; Bubbling fluidized bed; CFD-DEM

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. Modelling 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 modelling 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 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 modelling 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 modelling.

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

Table 1

Simulation conditions and parameters of the BFB and CFD-DEM model.

Bed size	0.27 x 1.05 x 0.001 m ³
Particle density	2600 kg/m ³
Particle diameter	0.001 m
Particle number	81000
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 x 105
DEM cells number	90 x 350
CFD time step	5 x 10 ⁻⁵ s
DEM time step	5 x 10 ⁻⁶ s
Particle normal stiffness	10000 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

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.

Table 2

Constitutive equations of CFD-DEM model: linear spring-dashpot model and inter-phase drag coefficient.

Particle contact force

$$\mathbf{F}_{ab,n} = -k_n \delta_n \mathbf{n}_{ab} - \eta_n \mathbf{v}_{ab,n} \quad \mathbf{F}_{ab,t} = -k_t \delta_t \mathbf{t}_{ab} - \eta_t \mathbf{v}_{ab,t}$$

$$\text{If } |\mathbf{F}_{ab,t}| > \mu_f |\mathbf{F}_{ab,n}| \text{ then } \mathbf{F}_{ab,t} = -\mu_f |\mathbf{F}_{ab,n}| \mathbf{t}_{ab}, \text{ and reset } \delta_t = |\mathbf{F}_{ab,t}| / k_t$$

Relative velocity, direction unit vector, and overlap

$$\mathbf{v}_{ab} = (\mathbf{v}_a - \mathbf{v}_b) + (R_a \mathbf{w}_a + R_b \mathbf{w}_b) \times \mathbf{n}_{ab} \quad \mathbf{v}_{ab,n} = (\mathbf{v}_{ab} \cdot \mathbf{n}_{ab}) \mathbf{n}_{ab} \quad \mathbf{v}_{ab,t} = \mathbf{v}_{ab} - \mathbf{v}_{ab,n}$$

$$\mathbf{n}_{ab} = (\mathbf{r}_b - \mathbf{r}_a) / |\mathbf{r}_b - \mathbf{r}_a| \quad \mathbf{t}_{ab} = \mathbf{v}_{ab,t} / |\mathbf{v}_{ab,t}|$$

$$\delta_n = R_a + R_b - |\mathbf{r}_a - \mathbf{r}_b| \quad \delta_t = \delta_n \sin \theta_t + \delta_n \cos \theta_t \Delta t \quad \delta_t' = \delta_t - (\mathbf{v}_{ab,t} \cdot \mathbf{t}_{ab}) \delta_t / |\mathbf{v}_{ab,t}|$$

Damping coefficient

$$\eta_n = 2\sqrt{m_{ab}k_n} \ln e_n / \sqrt{\pi^2 + \ln^2 e_n} \quad \eta_t = 2\sqrt{m_{ab}'k_t} \ln e_t / \sqrt{\pi^2 + \ln^2 e_t}$$

$$m_{ab} = (m_a m_b) / (m_a + m_b) \quad m_{ab}' = 2/7 m_{ab}$$

Ergun / Wen & Yu drag coefficient

$$\beta = \begin{cases} \frac{(1-\varepsilon_g)}{\varepsilon_g^2 d_p} \left(150 \frac{(1-\varepsilon_g)\mu_g}{d_p} + 1.75 \rho_g \varepsilon_g |\mathbf{u} - \mathbf{v}_p| \right) & \varepsilon_g \leq 0.8 \\ \frac{3}{4} C_D \frac{\rho_g |\mathbf{u}_g - \mathbf{v}_p| (1-\varepsilon_g)}{d_p} \varepsilon_g^{-2.7} & \varepsilon_g > 0.8 \end{cases}$$

$$C_D = \begin{cases} \frac{24}{Re} (1 + 0.15 Re^{0.687}) & Re \leq 1000 \\ 0.43 & Re > 1000 \end{cases} \quad Re = \rho_g \varepsilon_g |\mathbf{u}_g - \mathbf{v}_p| d_p / \mu_g$$

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][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 Table 1 and Table 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

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

where component $s_{nm}(t_c)$ contains the particle list in the state nm at time t_c .

The transition matrix $\mathbf{P}$ has the size of $(n \cdot m) \times (n \cdot m)$, and the entry p_{ij} represents transition probability that particles move from state i to state j . The proportion of the particles moving to state j from state i at time t_c calculated based on CFD-DEM result forms a transition probability $p_{ij}(t_c)$, and the transition probabilities between each two states at this time step constitute a transition matrix $\mathbf{P}(t_c)$. The average value of the matrixes of all transition time steps is the final transition matrix $\mathbf{P}$. So the development of the BFB system can be described as follows:

$$\mathbf{S}(t_{c+1}) = \mathbf{S}(t_c) \mathbf{P} \quad (2)$$

In this paper, m is set as 18, n is set as 42, and Δt is set as 0.025 s accordingly. The transition of particles from one cell to another is simulated by MCM using the transition matrix $\mathbf{P}$, but the particles distribution in a certain cell is totally random. The particle information obtained from the CFD-DEM result at time 15 s is the initialization of MCM.

2.3. Stochastic bubble developing model

Stochastic model is very different from the traditional CFD methods that based on the most basic rule and fundamental equations of physics or fluid dynamics. It is almost impossible to strictly testify the stochastic regularity of such complicated actual particle system as fluidized beds through mathematical methods. Stochastic model mostly focuses on the statistic regularity of groups instead of individuals and reproduces the group regularity by

stochastic behavior of individuals. Some adventurous but not unreasonable stochastic methods are necessary, as long as they are based on some mature macro-descriptions. The behavior of a single particle in fluidized beds seems to be unpredictable, but there is still some regularity to follow while a group of particles attract the attention. That is why stochastic modeling is a potential method to simulate this kind of system. And from a statistic and stochastic point of view, it is not appropriate to focus on the driving force or many other micro-dynamics of particle-fluid flow any more.

Simulating the statistic behavior of bubbles in bubbling fluidized beds and introducing their influence to the stochastic movement of particles are effective approaches to reflect the transient particle characteristics. Time-homogeneous MCM of particles has the advantage of intuitively describing macroscopic properties of granule systems, but the time-averaged trend it predicts hardly reflects bubble information (which is shown in section 3.2). SBDM is aimed to improve the shortcoming, which concerns the whole development processes of bubbles, including the generating, growing, moving and shaping. The stochastic concept is a leading thread throughout. A recommended way to obtain the bubble information for SBDM is the image recognition of visualizing CFD-DEM results.

Snapshots of CFD-DEM simulated results shown in Fig. 1 visually represent abundant information of bubbles. MATLAB is used to process all these snapshots from 10 to 15 s. Bubble appearing probability distribution can be obtained by graying, overlapping and averaging the intensity of all snapshots from 10 to 15 s, as shown in Fig. 2. Bubbles have high probability to appear in the middle of the bed, and as the bubble size generally increases with the rising, the range that bubbles appear becomes larger along the height of bed. Because

shapes of bubbles are various and unpredictable, an effective method to locate a bubble is to track its centroid. Through image graying and binaryzation process, the centroid coordinates and equivalent-area circle diameters of bubbles can be obtained by MATLAB.

2.3.1. Stochastic bubble generating sub-model

The bubble size is infinitesimal when generating from the bottom of the bed, so it is impossible to locate its centroid by image recognition. And just because of its infinitesimal size, the statistical bubble appearing probability distribution near the bottom of bed can represent the bubble generating probability distribution along the bottom of bed, as shown in Fig. 3. $\int f(w)$ is the cumulative probability distribution function of bubble generating. A Monte Carlo cumulative sampling method is applied to locate the bubble generating position w_0 in SBDM by a random number r_0 , which is generated by computer and ranges from 0 to 1, as shown in Eq. (3).

$$r_0 = \text{random}(0,1) = \int_0^{w_0} f(w) dw \quad (3)$$

Another important parameter in stochastic bubble generating sub-model is the bubble generating frequency. In SBDM, as the number of bubbles recognized from each snapshot is nearly invariable, the number of bubbles in the bed is assumed to be constant, which means when a bubble disappears, a new bubble will generate. The specific implementation is that the constant bubble amount is the average bubble number in one CFD-DEM snapshot at all time steps. While a bubble centroid reaches the upper edge of the bubble appearing probability distribution area (the light gray part of bed in Fig. 2), it is considered to disappear, and a new bubble centroid is generated according to Eq. (3) at the same time. The bubble information

obtained from the CFD-DEM snapshot at time 15 s is the initialization of SBDM.

2.3.2. Stochastic bubble moving and growing sub-model

Fig. 4 and Fig. 5 are the bubble centroid distribution in the BFB and the bubble diameter (equivalent-area circle diameter) distribution along the height of bed respectively. Based on the statistical data, the bubble centroid distribution range is limited by line 1 and line 2 in Fig. 4, and the bubble diameter changes within the range limited by line 3, line 4 and line 5. Assuming that the bubble centroid and diameter distribution within these two ranges are both even. Values $w_{t,1}$ and $w_{t,2}$ in Fig. 4 are the radial coordinates of intersections between $H = h_t$ and line 1 and between $H = h_t$ and line 2. So are the values in Fig 5. When a new generated bubble centroid is located at the bottom of bed, an initial height h_0 (1 cm) is given. Based on the even distribution assumption, d_0 is set to be a random number between $d_{0,3}$ to $d_{0,5}$ according to Fig. 5. The bubble rise velocity u_t is calculated using Davidson and Harrison [25] formula, as shown in Eq. 4. So the bubble centroid height h_{t+1} can be calculated as Eq. 5.

$$u_t = 0.71\sqrt{gd_t} \quad (4)$$

$$h_{t+1} = h_t + \Delta t \cdot u_t \quad (5)$$

$$w_{t+1} = \text{random}(w_{(t+1),1}, w_{t+1,2}) \quad (6)$$

$$d_{t+1} = \text{random}(\text{maximum}(d_{t+1,5}, d_{t+1,4}, d_t), d_{t+1,3}) \quad (7)$$

When the height h_{t+1} of a bubble centroid is obtained, the bubble centroid radial coordinate w_{t+1} and bubble diameter d_{t+1} can be calculated by the same stochastic method, as shown in Eq. 6 and Eq. 7. A basic principle is that the bubble diameter becomes larger and larger while rising, so the d_{t+1} is a random number between maximum ($d_{t+1,5}$, $d_{t+1,4}$, d_t) to $d_{t+1,3}$, which indicates the bubble coalescence is simplified to be part of the bubble growing, and

bubble breakage is not taken into consideration in the process of rising.

2.3.3. Stochastic bubble shaping sub-model

Based on the previous two bubble developing sub-models, the generating and moving of bubble centroid and diameter can be simulated. However, bubble shape is the key to couple bubble phase with particle phase. Fig. 6 shows an assumption of the typical spherical cap bubble model [26]. The main part of the bubble is the rest part of circle C_1 cut by circle C_2 . C_1 and C_2 have the same radius r_t , and the distance from C_2 center to C_1 edge is $r_t/2$.

The bubble is divided into two parts, region I (white part) and region II (light gray part). And the cut part of C_1 is marked as region III (dark gray part), which is in the position of bubble wake. The centroid of bubble is approximately set as the center of C_1 , and the equivalent-area circle radius of bubble is approximately set as the radius of C_1 . The initial particle position before coupling is calculated by MCM, and the bubble only has influence on the particles inside the three regions.

The coupling method between bubble phase and particle phase depends on in which region the particle is. If the particle position calculated by MCM is in region I, the coupling method is to move the particle out of the bubble along radial direction, as shown in Fig. 6. The distance to move depends on the original distance between the center of C_1 and particle position, which is calculated according to Eq. (8). And the edges of bed are certainly the limited baselines. Basically the closer that original particle position is to the center of C_1 in region I, the farther it is from the center after coupling, which is in line with Davison model [25]. The basic description of Davison model is that the particles above the bubble move upwards or obliquely upwards, the particles on the sides of bubbles move downwards, and the

particles in the wake of bubbles move towards the center of bubbles. To be applied here, there should be a negative correlation between the distance particle need to move and the distance from the particle to the related circle center. Anyway, there is still a random number range from 0 to 1 to control the unpredictable distance.

$$D_1' = r_t + \text{random}(0,1) \cdot (r_t - D_1)^2 / r_t \quad (8)$$

Considering the complicated swirls and entrainment phenomenon in the bubble wake, when the original particle position is in region II, the coupling method is to move the particle close to or into the bubble wake (region III) along the radial direction of C_1 . The distance to move is shown as Eq. (9).

When the original particle position is in region III, particle is moved away from the C_2 center and into bubble along the radial direction of C_2 . The distance to move is shown as Eq. (10).

$$D_{II}' = r_t - \text{random}(0,1) \cdot (r_t - D_{II})^2 / r_t \quad (9)$$

$$D_{III}' = r_t + \text{random}(0,1) \cdot (r_t - D_{III})^2 / r_t \quad (10)$$

What needs to be stressed is that the particle is coupled only with the closest bubble at one time step.

3. Results and discussion

3.1. Computing time

Fig. 7 shows the computing sequence and computing time of three models. SBDM and MCM are both initialized using CFD-DEM result at time 15 s, and the subsequent 5 s simulation costs CFD-DEM about 150 h, while it costs MCM only about 100 minutes and

SBDM coupled with MCM (SBDM-MCM) about 125 minutes. The stochastic model calculation is about 70 times faster than CFD-DEM, which is very efficient.

3.2. Particle distribution

Fig. 8a shows the snapshots of particle distribution calculated by CFD-DEM from 15 to 20 s under the fluidized air velocity of 1.5 m/s. In order to intuitively observe the trend of particle movement, particles are initialized with four different colors according to which region of the bed they are in at time 15 s. From the color distribution and how it changes over time, the particles are strongly mixed and flow upward in the middle of bed at first, and then spread and fall downward along the bed sides, which indicates the particle back mixing feature of BFB.

Fig. 8b shows the snapshots of particle distribution calculated by MCM in the same time period. The particle back mixing trend can also be observed by the same particle-colored method, which indicates MCM learns well from CFD-DEM in particle mixing trend. But a clear characteristic of MCM is the particle distribution is remarkable even, and no bubbles can be seen.

The SBDM-MCM calculated particle distribution snapshots are shown in Fig. 8c. The particle back mixing feature is also maintained well. Besides, the SBDM-MCM successfully presents the bubble structure in the snapshots, and the generating, growing and moving of bubbles can be clearly observed, just as the description of SBDM. The bubble coalescence and its impact on particle movement can also be observed.

3.3. Particle mixing

Detailed radial particle mixing curves of three models under the fluidized air velocity of 1.5 m/s are shown in Fig. 9a to furtherly compare the three models and state the importance of SBDM. Light green and purple particles in the left half bed (marked in section 3.2) are tracked to calculate their total number proportion of all particles over time. There are about 54% of the total particles in the left half bed at time 15 s, and after 5 s simulation, about half of them move to the right half bed. All three models show this same mixing trend. But the mixing speed of MCM is a little slower compared to the other two, and the mixing curve is very smooth, while both the CFD-DEM and SBDM-MCM calculated mixing curves show frequent and instantaneous undulation.

When the fluidized air velocity is raised to 1.8, 2.1 and 2.4 m/s, the radial particle mixing curves are respectively shown in Fig. 9b, Fig. 9c and Fig. 9d. The mixing cures of MCM continue to be very smooth and in the situation of the time-averaged particle mixing curves of CFD-DEM. The SBDM-MCM calculated mixing curves somewhat show similar fluctuation to the CFD-DEM calculated mixing curves.

Fig. 10a shows detailed axial particle mixing curves of three models under the fluidized air velocity of 1.5 m/s. Purple and dark green particles in the lower half bed (marked in section 3.2) are tracked to calculate their total number proportion of all particles over time. As the rising of bubbles makes great vertical disturbance to the particles nearby, especially the particles in bubble wake, the axial particle mixing is very strong, just as the violent waves displayed by CFD-DEM calculated axial mixing curve. Analogously, the axial mixing curve calculated by SBDM-MCM also fluctuates a lot. However, not only the axial mixing curve of MCM is smooth, but the particle proportion stabilizes near a certain value after a sharp

decline within about 1 s.

When the fluidized air velocity is raised to 1.8, 2.1 and 2.4 m/s, the axial particle mixing curves are respectively shown in Fig. 10b, Fig. 10c and Fig. 10d. Both the CFD-DEM and SBDM-MCM calculated particle proportions are varied in a comparatively large range after a sharp decline, while the MCM calculated particle proportions are stable after the first decline. The sharp-decline mixing curves at the beginning indicate the strong axial particle mixing in the BFB, which manifests as the color intersection of the upper and lower half bed particles. The later limited fluctuations of CFD-DEM and SBDM-MCM calculated mixing curves or stable mixing values calculated by MCM declare that the colors of the upper and lower half bed particles has been well blended, which is a relatively steady axial particle mixing status. Using the axial mixing curves at this status to discuss the disturbance caused by bubbles is more representative.

Table 3

The average particle proportions in the axial mixing curves from 17 to 20 s.

Fluidized air velocity, m/s	Average particle proportion, %		
	CFD-DEM	MCM	SBDM-MCM
1.5	40.07	48.49	45.47
1.8	35.72	42.51	35.61
2.1	21.99	23.00	22.04
2.4	20.94	23.41	20.65

Table 3 gives the average particle proportions in the axial mixing curves from 17 to 20 s, which are calculated by three models under four fluidized air velocities. A clear trend is that

the averaged proportions of the sum of purple and dark green particles in the lower half bed of total particles from 17 to 20 s decreases as the fluidized air velocity increases. It is easy to understand that the average voidage of the bed increases as the fluidized air velocity increases, which causes less particles in the lower half bed and more particles in the upper half bed. Besides, the average particle proportions calculated by MCM are notably larger than that calculated by CFD-DEM and SBDM-MCM under all four fluidized air velocities, while the SBDM-MCM results are much closer to the CFD-DEM compared to MCM. This indicates that the average voidage of BFB calculated by pure MCM is much smaller than the real value, and the calculated expansion ratio of bed is incorrect. The related SBDM-MCM results seem more reliable from Table 3, as the motion of bubbles is concerned.

In order to investigate the instantaneous impact strength caused by bubbles to the movement of particles, derivative particle proportions in axial particle mixing curves of three models under the fluidized air velocity of 1.5 m/s is shown in Fig. 11a. Same results under the other three fluidized air velocities are respectively shown in Fig. 11b, Fig. 11c and Fig. 11d. The small waves shown in the derivative axial particle mixing curves calculated by MCM indicate pure MCM of particles weakens the bubble impact on particle movement a lot. The periodical pulsations in SBDM-MCM calculated derivative axial particle mixing curves (especially in Fig. 11(d)) indicate the regular particle movement near the bubbles, as all bubbles in SBDM-MCM have the same spherical cap shape. Because the actual shapes of bubbles are changeable just as the CFD-DEM calculated particle distribution displays, the pulsations in CFD-DEM calculated derivative axial particle mixing curves are much more chaotic.

By comparing the particle mixing of three models, the result indicates the Markov process of particles learns the time-averaged particle movement well from CFD-DEM, but the instantaneous disturbance caused by bubbles cannot be reflected. However, the moving, growing, coalescence and breakage of bubbles do have strong impact on the movement of particles nearby. Mixing curves are improved a lot not just on the mixing degree but also pulsating characteristics while the motion of bubbles is simulated in SBDM-MCM, which strongly and distinctly illustrates the significance of coupling MCM with SBDM. However, the impact of the identically-shaped bubbles on particle movement reflected by SBDM-MCM is still not satisfactory compared with the CFD-DEM or the reality.

4. Conclusions

SBDM-MCM is introduced to model the particle movement in a 2D BFB. The results show this kind of stochastic model has extremely quick calculating speed compared with CFD-DEM, and has the ability to describe both macroscopic and microscopic particle movement characteristics. Especially the model successfully simulates the development and structure of bubbles, and introduces the effect of bubbles to the Markov process of particles, which improves the particles mixing a lot, and is very helpful and necessary for the future chemical reaction, mass transfer and heat transfer modelling.

Anyway, the bubble generating, moving, growing and shaping sub-models still need to be further developed and improved. The dependency to the statistical sample data is the major limitation of the proposed stochastic model, as the model cannot just change the entry condition to adapt to the change of operating condition, while CFD-DEM relatively shows strong adaptability. To find a way of easily adapting to the change of operating condition by

adjusting the transition matrix is a very challenging research for promotion of the stochastic model. And one of the potential developments of the stochastic model is to extend the dimensions or scale up the size of physical model by transforming the transition matrix according to the similarity of spatial particle movement in fluidized beds. That means the stochastic model might simulate a large 3D fluidized bed sampling from CFD-DEM results of a small 2D fluidized bed, which will save more time and computation demand compared to CFD-DEM. Besides, more samples from elaborate experiments are suggested to rich and support the model.

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
$\mathbf{P}$	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

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Figure captions:

Fig. 1. CFD-DEM simulated particle distributions in the BFB after $t = 10, 10.025, 10.05$ and 10.075 s. Fluidized air velocity: 1.5 m/s

Fig. 2. Statistical bubble appearing probability distribution in the BFB. Fluidized air velocity: 1.5 m/s

Fig. 3. Bubble generating probability distribution along the bottom of bed. Fluidized air velocity: 1.5 m/s

Fig. 4. Bubble centroid distribution in the BFB. Fluidized air velocity: 1.5 m/s

Fig. 5. Bubble diameter distribution along the height of bed. Fluidized air velocity: 1.5 m/s

Fig. 6. Diagram of bubble shaping model.

Fig. 7. Diagram of computing sequence and simulation time.

Fig. 8. Particle distribution comparison of three models. Fluidized air velocity: 1.5 m/s. (a) CFD-DEM; (b) MCM; (c) SBDM-MCM

Fig. 9. Proportion of the sum of light green and purple particles in the left half bed of total particles. Fluidized air velocity: (a) 1.5 m/s; (b) 1.8 m/s; (c) 2.1 m/s; (d) 2.4 m/s

Fig. 10. Proportion of the sum of purple and dark green particles in the lower half bed of total particles. Fluidized air velocity: (a) 1.5 m/s; (b) 1.8 m/s; (c) 2.1 m/s; (d) 2.4 m/s

Fig. 11. Derivative particle proportions in axial particle mixing curves of three models. Fluidized air velocity: (a) 1.5 m/s; (b) 1.8 m/s; (c) 2.1 m/s; (d) 2.4 m/s

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8 (a)

Figure 8 (b)

Figure 8 (c)

Figure 9 (a)

Figure 9 (b)

Figure 9 (c)

Figure 9 (d)

Figure 10 (a)

Figure 10 (b)

Figure 10 (c)

Figure 10 (d)

Figure 11 (a)

Figure 11 (b)

Figure 11 (c)

Figure 11 (d)