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A novel mixing index and its application in particle mixing behavior study in multiple-spouted bed

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ABSTRACT

Particle mixing is a very important process in many industrial reactors. It is important to consider how to quantify the particle mixing behavior accurately under different conditions. In this paper, the drawbacks of traditional mixing indexes, such as Lacey index are discussed, and then a novel particle mixing index, without grid dependency and particle color dependency was proposed based on the neighbor distance method and coordination number concept. Its characteristics such as parameters selection, calculation method and multi-direction were discussed in details. The proposed mixing index was used for investigating particle mixing behavior in the multiple-spouted bed under conditions of different gas velocity ratios and different particle density ratios. The experimental results have been used to validate the simulation results at first. It is found that the improved mixing index is more superior and effective compared with the traditional mixing index methods, and suitable for the investigation of particle mixing behavior. It was indicated that the density ratio is a key factor to influence particle mixing process. The novel particle mixing index without grid dependency and particle color dependency is recommended to study particle mixing behavior in other particulate processes in the future.

1. Introduction

Spouted bed is a widely used chemical reactor for processing coarse particles since it was invented in 1955 [1]. It has been widely used in various physical operations such as coating [2, 3], drying [4, 5], pyrolyzing [6, 7], granulation [8, 9] and combustion [10, 11]. To satisfy different purposes of industrial production and achieve optimum productivity, spouted bed has been developed to many kinds of designs such as rotating spouted bed [12, 13], conical spouted bed [14, 15], spout-fluid bed [16, 17] and multiple-spouted bed [18–20]. Among them, the multiple-spouted bed has drawn many attentions, because of larger capacity, better gas-solid contact efficiency, higher rate of mass and heat transfer. There have been a few literatures on the multiple-spouted bed.

In previous studies, Maureen [21] has experimentally investigated the multiple rectangular spouted bed using the PIV/PEPT technology, and simulated particle behaviors using the discrete particle model (DPM) method. The flow pattern map and distribution of the average particle velocity was obtained. A recent investigation on the particle flow patterns and transitions in the multiple-spouted bed was reported [18]. It was found that flow patterns can be described as fixed bed (FB), internal jet (IJ), internal jet with bubble (IJB), single spouting (SS), multi-spouting (MS) and internal jet with slugging (IJS) based on typical flow pattern images of the multiple-spouted bed. Some characteristics of the spouting process such as minimum spouted velocity and pressure drop were also given. The hydrodynamic characteristics in the multiple-spouted bed was simulated using two-fluid model [19], which was compared with experimental results [18]. The influence of the ratio of central/auxiliary gas velocity on the hydrodynamic characteristics such as spouting height, spouting area and flow patterns was studied. Recently, the multiple-spouted bed was used to coat nuclear fuel particles. Particle densities varied significantly, from 13.8 g/cm^3 to 5.6 g/cm^3, in the whole coating process [22], so it is necessary to study the effect of density ratio on the particle flow patterns.

Both experimental approach and numerical method can be used to investigate characteristics of the particle and fluid flow in the multiple-spouted bed. Experiments can provide substantial insights into the flow characteristics in lab-scale multiple-spouted bed, but their expensive cost and complex operation restrict their wide application in the research. In recent years, with rapid development of numerical computational techniques and high-performance computers, numerical simulation with computational fluid dynamics (CFD) is used widely to obtain detailed information of the flow characteristics in the multiple-spouted bed. The numerical simulation has proved to be a powerful tool to bridge the gaps between theoretical analyses and experiments [23].

Particle mixing behavior has also been paid many attentions in spouted bed research, because it relates to particle utilization efficiency directly, and also can be linked with the dispersion coefficient of the chemical reactor. Recently, the characteristic mixing time of solids which based on the Lacey method was used to linked with the lateral

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dispersion coefficient in bubbling fluidized beds [24]. Besides, particle mixing behavior is also an important research field in kinds of particle processing equipment, such as rotating drum [25, 26], plowshare mixer [27, 28] and ribbon mixers [29, 30]. So how to quantify the particle mixing behavior accurately should be considered carefully. Mixing index should be defined for the quantitative characterization of the particle mixing degree, which can be calculated via many different methods, such as average height method, Lacey method and sphere spreading method in previous literatures [31].

Zhang et al. [32, 33] investigated particle mixing in flat-bottom spout-fluid bed by experiment and DEM simulation respectively. It was found that particle mixing process could be divided into three sequential stages of macro-mixing stage, micro-mixing stage and stable mixing stage, and the convective mixing, shear mixing and diffusive mixing were three different mixing mechanisms in spout-fluid bed. Zhu et al. [34] investigated the mixing characteristics of the dry and wet particles in a rectangular spouted bed, and the Ashton mixing index was adopted to evaluate the dynamic mixing process of the particle system. You et al. [35] investigated the packing and flow behavior of ellipsoidal particles by DEM simulation and experiment respectively. Some experimental validations of the Lacey mixing index for particle mixing process have been conducted. The mixing index increases from 0 to around 1 as time increases, and the simulation results are in good agreement with the experimental results. Xiao et al. [36] did some experimental and DEM research on the particle mixing performance in rotating drums, and the validity of the DEM simulations was confirmed by comparing the numerical results with the experimental ones. Ren et al. [37] investigated the mixing behaviors in a spouted bed with different density particles using discrete element method. The mixing process, evaluation of mixing quality, particle circulation and distribution of particle concentration along both radial and axial directions were obtained on the basis of simulations. And the mixing process was illustrated by the development of solid flow patterns with time. Takabatake et al. [38] applied the coarse-grain model to investigate mixing state in a spouted bed. It was found that the mixing state well agreed between the original and coarse grain particle systems, and the coarse-grain model made it possible to reduce the calculation cost drastically. Besides, Tamadondar et al. [39] and Gui et al. [40, 41] investigated adhesive particle mixing, tetrahedral particle mixing and motion in rotating drums and cubic particle mixing patterns in a three-dimensional cylinder respectively.

Solids mixing index is an important parameter in binary mixtures fluidization, which gives a reflection of the mixing or segregation state in fluidization [42]. Various mixing indexes, essentially based on statistical analyses, are employed to describe the solid mixing in many different industrial processes [43]. Traditionally, Lacey method and mixing entropy method was used most widely, but its disadvantage is obvious because of its grid and particle color dependency. For one particle mixing state, the mixing index may be different if different grid was chosen. So, some new methods to quantify the particle mixing are proposed: nearest neighbor method and neighbor distance method [31]. The particle-scale index method was suggested for calculating the mixing index recently [30, 44]. It is based on the combination of the coordination number and the Lacey method. The effectiveness of newly proposed mixing index was validated with DEM simulation for different parameters [30]. Also, a new method was developed to determine the mixing degree, which is based on the relative position change of every two particles, and the calculating results with different shapes and sizes of mixing space were analyzed [45].

The paper was organized as follows. The numerical simulation method was described at first, then an improved method for calculating the mixing index without particle color dependency and grid dependency was proposed, and its characteristics were discussed in detail. The newly improved mixing index was used for the investigation of multiple-spouted bed based on CFD-DEM simulations, which were also validated by experimental results. And then the influences of gas velocity ratio and particle density ratio on particle mixing behavior have been studied. Some conclusions were drawn at last.

Table 1
Relevant physical equations used in Hertz-Mindlin model.

Variables	Equations
For Normal forces	$\mathbf{F}_n = \mathbf{F}_n{}^s + \mathbf{F}_n{}^d$
Normal spring force	$\mathbf{F}_n{}^s = -k_n \boldsymbol{\delta}_n^{\frac{3}{2}}, \quad k_n = \frac{4}{3} Y^{eq} \sqrt{R^{eq}}$
Normal damping force	$\mathbf{F}_n^d = -2\beta\sqrt{\frac{5}{4} k_n m^{eq}} \boldsymbol{\delta}_n{}^{\frac{1}{4}} \mathbf{v}_n^{rel}, \quad \beta = \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}}$
For tangential forces:	$\mathbf{F}_t = \begin{cases} \mathbf{F}_t^s + \mathbf{F}_t^d, \text{if } \lvert\mathbf{F}_t\rvert \le \mu_s \lvert\mathbf{F}_n\rvert \\ -\mu_s \mathbf{F}_n, \text{if } \lvert\mathbf{F}_t\rvert > \mu_s \lvert\mathbf{F}_n\rvert \end{cases}$
Tangential spring force	$\mathbf{F}_t{}^s = -S_t \boldsymbol{\delta}_t, S_t = 8G^{eq}\sqrt{R^{eq}\delta_n}$
Tangential damping force	$\mathbf{F}_t^d = -2\sqrt{\frac{5}{6}}\beta\sqrt{S_t m^{eq}} \mathbf{v}_t^{rel}, \quad \beta = \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}}$
Interparticle torque	$\boldsymbol{\tau}_c = -\mathbf{R} \times \mathbf{F}_t^s$
Rolling friction torque	$\boldsymbol{\tau}_r = -\mathbf{R} \times \mathbf{F}_t^d$

2. Numerical simulation

2.1. CFD-DEM method

Discrete element method (DEM) is a numerical method for computing the motion and interaction of discrete interacting bodies. The movement behavior of single particle and the collision process between particles can be simulated to obtain the velocity and position of particles at any time by DEM. The core of the method is how to choose the appropriate contact force model. As we know, when two particles collide, they actually deform. However, the overlap displacement is assumed rather than considering deformation in the soft sphere model. Besides, the larger displacement results in the larger repulsive force. Particles will lose kinetic energy because of such a particle-particle interaction. For the normal force, it has a spring which provides the repulsive force and a dashpot that provides the inelasticity in the collision. For the tangential force, it has a spring modelling tangential elastic deformation of the contacting surfaces and a dashpot modelling plastic deformation respectively. The tangential force, which can be withstood by the contact before one particle's sliding, is limited by the Coulomb friction. Considering the above all kinds of mechanisms, the Hertz-Mindlin model is chosen to describe the collision between particles in the study as shown in Table 1 [46].

In Table 1, Y^{eq}, R^{eq}, m^{eq}, δ_n, δ_t, S_n, S_t, μ_s, μ_r, $\mathbf{R}$ are the equivalent Young's Modulus, the equivalent radius, the equivalent mass, the normal particle overlap, the tangential particle overlap, the normal stiffness, the tangential stiffness, the coefficient of sliding friction, the coefficient of rolling friction and the radius vector respectively. β is the damping factor, which is a function of the restitution coefficient e. The restitution coefficient can be determined experimentally. A detailed description of the model parameters is omitted here and can be found in any literatures describing the Hertz-Mindlin model.

The CFD-DEM coupled model can be used to simulate the gas-solid two-phase flow [47]. In the coupled model, the local averaged Navier-Stokes equations describe the gas flow and the motion of particles can be obtained through Newton's second law and rotation equation. The coupling theory and the specific method of CFD-DEM model can be referred to previous literature [48, 49].

The CFD-DEM simulation scheme is shown in Fig. 1. First of all, the flow field of the gas phase is resolved by the CFD solver and transferred to the coupling module when a stable solution is obtained. In the coupling module, the drag force can be obtained when the relative velocity difference between each particle and its surrounding gas has been calculated. Then the drag force acting on each particle is transferred to the DEM solver where the particle properties such as positions will be updated. The fluid cell porosities and the momentum sink term for each mesh cell will be calculated when the new particle properties are