Chemical Engineering Science 65 (2010) 3034–3041

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

A macroscopic and microscopic study of particle mixing in a rotating tumbler

Nan Gui, JianRen Fan *, Kefa Cen

State Key Laboratory of Clean Energy Utilization, Zhejiang University, Hangzhou 310027, PR China

ARTICLE INFO

Article history:
Received 21 October 2009
Received in revised form
20 January 2010
Accepted 22 January 2010
Available online 4 February 2010

Keywords:
Mixing
Particle
Granular materials
Numerical analysis
Macroscopic/microscopic
Information entropy
Discrete element method

ABSTRACT

The microscopic and macroscopic mixing of granular particles in a two-dimensional rotating tumbler is studied using the discrete element method (DEM). For microscopic study, a dimensionless function $\xi(c_a, c_b)$ is proposed to evaluate the degree of mixing of particles on the scales of particle size. It is demonstrated that the mixing interface is exponentially increased when the measurement scale decreases. Thus, a fractal structure of the mixing interface is indicated. By numerical analysis on the dimension of the interface, it is indicated that with the same rotations, a slow rotation speed is positive to particle mixing. Moreover, under the same time, there always exists a limit state under which the mixing is fully developed.

On the other hand, by calculating the mean auto- and cross-radial distribution functions, the mixing dynamics is evaluated based on a macroscopic point of view. By the radial distribution functions, a Shannon entropy-based numerical analysis is carried out. It is indicated that, analogical to theory of thermodynamics, the mixing is an information entropy-increased process, and the level of mixing is well evaluated by the value of Shannon entropy. Moreover, the increase process for the Shannon entropy is oscillated during the transition from one state in 'equilibrium' to another. The frequency analysis indicates the close relationship between the oscillation in entropy and the external effects, such as the rotational acceleration of the tumbler.

1. Introduction

The rotating tumbler is commonly used for mixing of materials, and a vast number of researches have been devoted to investigation of particle mixing in rotary tumblers during the past decades, either theoretically or experimentally. For early study of particle mixing in tumbler, Rajchenbach (1990) implemented a study on the flow of granular material under gravity, and showed the exhibition of either intermittent avalanches or a steady regime. Moreover, he established a relationship between the current and the slope which correspond to the transition from the discrete to the steady regime. Metcalfe et al. (1995) described a geometric technique for the analysis of slow granular mixing processes. They demonstrated the mixing behavior of particles in slow flow can be divided into geometric and dynamic parts, and the geometric aspect dominates for mono-disperse and weakly cohesive particles.

After that, many studies were carried out focusing on the mixing phenomenon in rotary tumblers or cylinders. For example, with regard to the de-mixing process caused by the differences in particle size and density, Boateng and Barr (1996) proposed a model to predict the preferential movement of particles in the shearing layer of a rotary kiln. Their result is available for assessing the effect of segregation on bed temperature nonuniformities in rotary kilns. Choo et al. (1997) observed a dynamical state that precedes the axial segregation in bidirectional traveling waves in a long drum mixer, and found the wave speed decreases with wavelength. Wightman et al. (1998) carried out a simulation of particle flow and mixing in a rotating and rocking cylinder. They compared the rotational motion with rocking to purely rotational motion, and showed the rocking motion can dramatically enhance the mixing. Shinbrot et al. (1999) reported the observation of spontaneous chaotic granular mixing patterns in a simple cylindrical tumbler partially filled with sufficiently fine grains. They identified the mechanism for the spontaneous patterns: a periodic stick-slip behavior occurred in the shear layer separating static and flowing regions of grains, which can cause weakly cohesive grains to mix at rates overwhelmingly exceeding those achievable for freely flowing grains.

More recently, McCarthy et al. (2000) gave a review on the numerical study of tumbler mixing, focusing on two different techniques, and discussed mixing and segregation in different tumbler geometries. Nase et al. (2001), McCarthy (2003) and Li and McCarthy (2005) carried out studies on the effect of cohesion between grains which is of the predominant mode due to interstitial liquid. Nase et al. (2001) proposed two characterization criteria in both static and flowing systems; McCarthy (2003) showed cohesion may increase the rate of mixing in tumbler

* Corresponding author. Fax: +86 571 87991863.
E-mail address: fanjr@zju.edu.cn (J. Fan).

0009-2509/$ - see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ces.2010.01.023

devices, and Li and McCarthy (2005) developed a particle-level model for accurately predicting the extent of particle mixing and segregation in cohesive granular system. Moreover, Alexander et al. (2006) studied the avalanching dynamics of particles and characterized the different dynamics of cohesive forces. Chaudhuri et al. (2006) studied the cohesive effect on mixing and segregation of binary mixtures in a rotating drum, and showed different effects of cohesion on the mixing patterns and rates. Kwapinska et al. (2006) used the DEM to simulate the transverse mixing of freely flowing particles in a two-dimensional rotating drum. They discussed the mixing times and numbers for different drum diameters, loadings, rotational frequencies and particle sizes, etc. They pointed out the necessity to replace the penetration models by DEM approaches to investigate systemically the various aspects on drum mixing. Cleary and Sinnott (2008) used DEM to better understand flow dynamics and assess mixing in devices of gravity controlled, bladed and high shear depending on the relative contribution of gravity and internal agitation. These classifications depend on the generation of the flow patterns that promote mixing. Arntz et al. (2008) studied the mixing and segregation of bidisperse granules in a rotating short cylindrical drum using DEM, focusing on the influence of fill level and angular velocity of the drum on the radial segregation patterns. They used a method based on the local entropy of mixing calculated by Boltzmann expression to quantify the local degree of mixing (a similar definition is also used by Finnie et al. (2005)).

In addition, Bertrand et al. (2005) discussed the recent state of art in the modeling of granular flows in mixing processes. They reviewed both the continuum and discrete-element-based models, concentrating on the discrete element method. Both the theoretical and the practical aspects of the DEM were addressed, as well as some new ideas on simulation of more complex mixing systems. With regards to the more complex system with heating effects, Figueroa et al. (2009) used a multi-scale, multi-physics modeling technique, i.e. Thermal Particle Dynamics (TPD), to examine the interplay between transient heat transfer and particle mixing in rotating tumblers. They studied the effect of the mixing rate on the heating rate of granular material by changing the rotation rate and the filling level. In their study, the Peclet and Nusselt number are used to determine the heating mechanism and the rate of heat transport, respectively.

On the other hand, for experimental study, Sherritt et al. (2002) gave an extensive review on experimental results of axial dispersion in the three-dimensional mixing of particles obtained in rotary kilns. After that, they proposed a new design equation for the axial dispersion coefficient in terms of rotating speed, degree of fill, drum diameter and particle size. They obtained the design correlations for slumping, rolling/cascading and cataracting bed behaviors by data points from the literature and validated the correctness of it by new measurements. Santomaso et al. (2004) carried out an experimental investigation on mixing of non-ideal powders in rotating batch cylinders under rolling regime, charactering and quantifying the local mixture composition by a solidification and image analysis coupling technique. They suggested a mixing mechanism of non-ideal granular material where convection plays a leading role.

Based on the aforementioned work, it is obvious that the mixing of granular particles in rotating tumblers is a fundamental subject for both the scientific and engineering studies. It is attracting significant interests of many researchers both theoretically and practically. Thus, the present study was carried out to improve the knowledge regarding the mixing of particles based on either the macroscopic or the microscopic viewpoints. This work used the discrete element method (DEM) to simulate the particle motion in the rotating tumbler. However, different from previous studies, the present study uses a microscopic study on the structure characteristics of mixing interface by a measuring function based on the local concentration of particles; whereas it uses a macroscopic study on the overall level of mixing degree by using the Shannon information entropy based on the radial distribution function. The numerical analysis is started from two preliminary separated parts of monoparticles. Then, the microscopic and macroscopic characteristics of mixing are analyzed based on the fractal dimension analysis and Shannon entropy analysis, respectively.

2. Numerical approach

2.1. Discrete element method

In the present study, the particle motion in the tumbler is tracked individually under the Lagrangian frame through solution of the Newton's equation of motion, and the particle–particle collision is simulated by the discrete element method in a deterministic way. The discrete element method is present state of the art of numerical simulation of granular dynamics. The soft-sphere approach, belonging to the DEM, was firstly proposed by Cundall and Strack (1979) and developed in simulation of fluidized bed by Tsuji et al. (1993). The soft-sphere model is mainly characterized by taking into account three basic aspects of inter-particle collision mechanism: elastic collision (modeled by a spring coefficient k and a restitution coefficient e), viscous damping effect (modeled by a damping coefficient β), and friction or sliding trends effect (modeled by a friction coefficient γ). Thus, it is of the form

$$m_p\ddot{\boldsymbol{x}} = \boldsymbol{f}_c = -k\boldsymbol{x} - \beta\dot{\boldsymbol{x}} \tag{1}$$

$$\text{If } |\boldsymbol{f}_c \bullet \boldsymbol{t}| > |\boldsymbol{f}_c \bullet \boldsymbol{n}|, \text{ then } |\boldsymbol{f}_c \bullet \boldsymbol{t}| = \gamma|\boldsymbol{f}_c \bullet \boldsymbol{n}| \tag{2}$$

where m_p, $\boldsymbol{f}_c$ and $\boldsymbol{x}$ are the particle mass, the contact force and inter-particle displacement respectively. '$\bullet$' denotes the time derivative, and $\boldsymbol{t}$ and $\boldsymbol{n}$ denote the tangential and normal directions between a pair of colliding particles, respectively.

Based on the Newton's law of motion, the particle translational ($\boldsymbol{u}_p$) and rotational motion ($\boldsymbol{\omega}_p$) of any particle is governed by

$$\dot{\boldsymbol{u}}_p = \frac{\boldsymbol{f}_c}{m_p} + \mathbf{g} \tag{3}$$

$$\dot{\boldsymbol{\omega}}_p = \boldsymbol{T}_p / I_p \tag{4}$$

where $\boldsymbol{f}_c$ for particle in the tumbler, and $\mathbf{T}_p$ and I_p denote the torque and the moment of inertia, respectively. In Eq. (3), the $\boldsymbol{g} = \binom{0}{g}$, where g is acceleration of gravity which only works in the vertical direction.

Initially, the tumbler is partially filled with spherical granular particles settled at the bottom. Then the tumbler rotates with the rotating angular velocity gradually increased until it reaches a target speed (the rotating acceleration is $\dot{\omega} = \pi\,\text{rad/s}^2$). We simulated several typical rotation speeds, which ranges from ω=0.5 to 3.0 rad/s. A sufficient fine time step of dt=1 μs is used to stabilize the simulation of particle motion. For clarity, the parameters used in the simulation are listed in Table 1 (the grid size in Table 1 is just used in simulation for necessary record of local collision information between particles, not used for the following fractal analysis of the mixing interface.)

2.2. Some definitions

2.2.1. Mixing measurement function

For the convenience of mixing study, we preliminarily divided the particles into two separate and equal parts by a vertical