CHEMICAL ENGINEERING RESEARCH AND DESIGN 91 (2013) 1646–1659

Contents lists available at ScienceDirect

Chemical Engineering Research and Design

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

Collective dynamics modeling of polydisperse particulate systems via Markov chains

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ABSTRACT

This paper develops an efficient approach to modeling and analyzing the overall dynamics of polydisperse particulate systems, exemplified using a rotating drum with horizontal axis, under both constant and time-varying operating conditions. This approach captures the collective dynamics using stochastic models in the form of Markov chains. The characteristics of such dynamics can be obtained from the Markov chains operator. It provides a systematic way to the analysis of collective dynamical features of particle movements. The obtained operators are used to estimate the spatial particle distribution and the degree of particulate mixing as examples of collective dynamic features of polydisperse particulate systems. In this paper, Markov chains models were developed from discrete element method simulation results to show the effectiveness of the proposed approach.

Keywords: Polydisperse particulate systems; Collective dynamics; Markov chains; Time-varying operations

1. Introduction

Particulate mixing is one of the most important industrial processes, especially in mining, pharmaceutical and chemical industries. Rotating drums with horizontal axis are common tools used for this process. An experimental based study of particle mixing–demixing behaviors in a rotating drum is reported in Abouzeid and Fuerstenau (2010). Mixing dynamics characterization of polymer powders using texture analysis is presented in Gosselin et al. (2008). The experimental study of granular mixing mechanism in drum mixers via digitized image analysis can be found in Santomaso et al. (2004). These experimental studies provide qualitative approaches to studying particulate mixing. However, these approaches cannot capture quantitatively the overall dynamics of particulate mixing, referred to as the collective dynamics in this work. It is difficult in general to model such collective dynamics in particulate mixing due to the highly complex particle interactions (Abouzeid and Fuerstenau, 2010; Santomaso et al., 2005), including the interactions between particles and between particles and the system boundary, e.g., the drum wall.

Numerical simulation approaches, such as the discrete element method (DEM), have been used to study particulate systems (Yang et al., 2000, 2003). The DEM can provide detailed microscopic information such as particle trajectory, velocity, and forces acting on each particle at any time during the process. Such information is difficult to obtain from experiments. In Arntz et al. (2008), DEM approaches were used to link particle behaviors (such as mixing and segregation) and operating parameters (such drum rotational speeds and filling level). A study of particle mixing, based on the DEM, using the dimension and entropy analysis is presented in Gui et al. (2010). The DEM was also used to study longitudinal and transverse particle mixing in rotary kilns (Finnie et al., 2005). However, DEM simulations can be very computationally complex, particularly for systems consisting of a large number of particles over long process durations (Finnie et al., 2005; Doucet et al., 2008). While the collection of the detailed information on individual particles from the DEM can form the collective behavior of all particles, a DEM model itself is not a direct model for the collective dynamics, and is far too complicated to be used for this purpose. This motivates the development of

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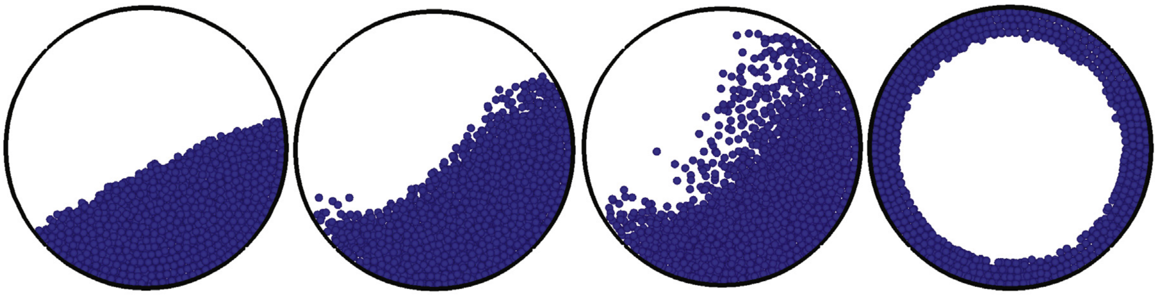
Received 18 December 2012; Received in revised form 3 May 2013; Accepted 14 May 2013
0263-8762/$ – see front matter
http://dx.doi.org/10.1016/j.cherd.2013.05.011



(a) Rolling regime (b) Cascading regime (c) Cataracting regime (d) Centrifuging regime

Fig. 1 – Flow regimes for 2000 particle system.

alternative modeling approaches to study collective particulate behaviors.

Stochastic approaches, for example Markov chains, have been used to study and analyze the collective dynamical features of particulate systems, such as particulate mixing. A Markov chains approach was used in particle mixing study in a motionless/static mixer (Chen and Fan, 1972; Ponomarev et al., 2009). This approach was also used to study particulate mixing in a hoop mixer (Aoun-Habbache et al., 2002) and rotary shear (Rippie and Chou, 1978). However, these experiment-based methods only give coarse qualitative estimations and often do not capture sufficient details in the collective dynamics. In Doucet et al. (2008), DEM simulations were used to generate particle trajectories to construct Markov chain operators. The operators were used to estimate the mixing evolution of monodisperse particulate systems (i.e., systems where all particles have the same properties) under constant operating condition.

Markov chain operators were adopted in our recent work (Tjakra et al., 2012) to characterize operating flow regimes and to estimate the spatial particle distribution, and more recently, to study particulate mixing of monodisperse particulate systems under time-varying operating conditions (Tjakra et al., 2012). This paper extends the above Markov chains based methods and develops an approach to modeling and analyzing the collective dynamic features of polydisperse particulate systems, with both constant and time-varying operating conditions (in particular, drum rotational speeds). This is a systematic and quantitative approach, different to the existing qualitative analysis, e.g., flow regimes based on observation of images particles. The Markov chains models can be developed for polydisperse particulate systems from DEM simulations or, alternatively, experimentally using from tracer methods such as positron emission particle tracking or particle measurement sensoring (Parker et al., 1997; Barigou, 2004; Zhang et al., 2009; Yang et al., 2008b). The proposed approach is not meant to be a replacement of but rather a complement to DEM simulations. The ultimate objective of the work is to develop an approach for industrial applications to which the DEM cannot be applied due to prohibitive computing cost or difficulties in obtaining DEM models. In this paper, DEM simulation results are used to construct Markov chain operators to demonstrate the effectiveness of the proposed approach. For illustrative purpose, the operators are used to estimate the evolution of collective dynamical features, including the spatial particulate distributions and the degree of particulate mixing. The proposed approach can be extended and applied in process optimization and eventually on-line control.

This paper is organized as follows. The collective dynamical features of particulate systems are reviewed in Section 2. Brief background of the DEM, stochastic systems, and Markov chains theory is presented in Section 3. In Section 4, the proposed Markov chains modeling for polydisperse particulate systems under both constant and time-varying operating conditions are presented. The collective dynamic features analysis from the Markov chain operator is presented in Section 5. Conclusion and future investigations are discussed in Section 6.

2. Collective dynamical features of particulate systems

Collective dynamical features of particulate systems in horizontal rotating drums are often qualitatively classified into different types of flow regimes. The commonly encountered flow regimes are rolling, cascading, cataracting and centrifuging regimes (Henein et al., 1983), as shown in Fig. 1. Many industrial processes are required to operate under a specific flow regime to meet product specifications (Mellmann, 2001). Particulate mixing is a common operation in pharmaceutical and mineral processing industries, often using a horizontal rotating drum. The basic phenomena for particulate mixing are still not fully understood and thus it is difficult to optimize mixing operations. If the mixing unit is not properly designed and operated, it may lead to undesired particle segregation (Arntz et al., 2008). The quality of mixing process is greatly affected by particulate trajectories and operating flow regimes (Santomaso et al., 2005). Mixing processes are typically operated under rolling, cascading or sometimes even in cataracting flow regime depending on the particulate properties. Mixing processes can be enhanced by alternating the operating flow regime (Santomaso et al., 2005; Arntz et al., 2008), hence justifying the proposed time-varying operations.

3. Methodology

Particulate systems typically involves a large number of particles, where each particle behavior such as translational and rotational motions, can be studied based on Newton's second law of motion. The collective dynamic behavior of particulate systems are highly complex due to the interactions between particles and also interactions with the system boundary. Discrete element method (DEM) simulations are used to generate particle trajectory information by solving the differential equations obtained from Newton's law of motion (Yang et al., 2008a; Moreno-Atanasio and Ghadiri, 2003; Mishra, 2003; Yu, 2004; Morrison and Cleary, 2004; Cleary, 2001). The DEM model used in this work is a 3D horizontal rotating drum with parameters given in Table 1. The construction of Markov chain