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Discrete element method based analysis of mixing and collision dynamics in adhesive mixing process

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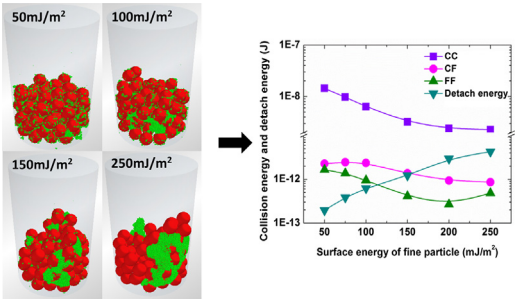
HIGHLIGHTS

- Adhesive mixing dynamics investigated via DEM using statistically significant number of coarse particles.
- Mixing dynamics analyzed through normalized fine-fine and coarse–fine contacts.
- Mixing quality was assessed via two parameters which capture mixing and coating quality.
- When collision energy is greater than detachment energy, collision rate determines mixing quality.
- Experimental results validate adhesive mixing dynamics attained in simulations.

GRAPHICAL ABSTRACT

Adhesive mixture quality impacted by the interplay between the collision energy and detachment energy as a function of surface energy of fine particles.



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ABSTRACT

When small amounts of fine particles are mixed with coarser particles, they tend to form ordered or adhesive mixtures. In order to understand the effect of fine particle amount and cohesion on the adhesive mixing process, discrete element method (DEM) simulations are carried out in which cohesion is represented by surface energy. High-intensity vibrational mixing was used to examine two important and related dynamic processes; fine particle deagglomeration and their subsequent adhesion to coarse particles, by analyzing normalized fine-fine (FF) and coarse–fine (CF) particle contact numbers, respectively, along with the mixing quality. It is found that FF contacts decreases with the mixing time, indicating deagglomeration, before reaching equilibrium; while CF contacts, an indicator of coating, as well as mixing quality increase before reaching equilibrium. A major new finding is that the number of fine particles per coarse particle at equilibrium follows lognormal distribution. The time scales to reach equilibrium FF contact number and mixing quality are comparable, indicating that deagglomeration is the dominant factor for achieving a uniform adhesive mixture. As expected, increasing surface energy of fine particles leads to decreased mixing quality due to stronger agglomerates that cannot be broken by collisions. On the other hand, collision rate can dictate mixing quality, as long as the collision energy is greater than the corresponding detachment energy of fine particles agglomerates. Selected experimental results validate the DEM simulations and their ability to describe the adhesive mixing process.

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1. Introduction

When coarse particles are mixed with a small amount of fine particles, the fine particles tend to adhere to the surface of coarse particles due to various adhesive forces, such as van der Waals, electrostatic, capillary and/or mechanical forces (Travers and White, 1971). Such mixtures are called ordered mixtures (Hersey, 1975), although that term is as been generally less used in favor of the term adhesive mixture (de Boer et al., 2012; Staniforth, 1987). Ordered mixtures, or adhesive mixtures are different from random mixtures because interparticle attractive forces in conjunction with particle size disparity play an essential role during the mixing process.

It has been reported that in ordered mixtures or adhesive mixtures, the distribution of fine particles within the sample of interest is uniform and even better than theoretical predictions based on random mixing theory (Buslik, 1973; de Boer et al., 2012). In addition, adhesive mixtures can also reduce or prevent subsequent segregation of particle components (Aulton and Taylor, 2013). Therefore, adhesive mixtures are widely used for improved mixing quality in the pharmaceutical industry, where mixture uniformity is of paramount importance when one constituent is much smaller compared to another (Bryan et al., 1979; Crooks and Ho, 1976; Huang et al., 2017; Kaialy et al., 2012; Saharan et al., 2008). Although many experimental papers have been published on adhesive mixtures, they mainly focus on the physicochemical properties of the particles and their effects on mixing homogeneity, not on dynamics of the mixing process (de Boer et al., 2012; Hooton et al., 2006; Jones et al., 2008; Jones et al., 2007; Kaialy, 2016; Le et al., 2012a; Saint-Lorant et al., 2007). For example, the ratio of the cohesive forces between fine particles to the adhesive forces between fine and coarse particles, i.e. Cohesive-Adhesive Balance (CAB), is considered to be an important factor, but the importance of CAB and its influence on process dynamics remains largely ignored (Begat et al., 2004a; Begat et al., 2004b).

In the adhesive mixing process, four different simultaneously occurring mechanisms are involved: (i) random mixing, (ii) deagglomeration, (iii) adhesion, and (iv) redistribution and exchange (de Villiers, 1997; Nguyen et al., 2015a). To optimize the overall process of adhesive mixing, it is necessary to understand these mechanisms. So far, however, compared to the intense research focusing on the effect of material properties on mixing performance, only limited information is available on their effect on different mechanisms and mixing dynamics (de Boer et al., 2012). As an exception, in a recent work, laser diffraction technique and non-destructive image analysis has been used to investigate the mixing dynamics, demonstrating the mixing time to get a uniform adhesive mixture is dictated by deagglomeration (Nguyen et al., 2015a). However, better understanding of the correlations between different mechanisms and the effect of material properties on adhesive mixing process have not been well investigated, and modeling of mixing process dynamics remains underexplored.

DEM simulations can track the evolution of particle assembly by computing the coordinates, velocities, forces, and torques of individual particles in the system. This information from DEM simulations can be analyzed as a function of simulation time and can provide information relevant to the dynamic behavior. In recent years, DEM simulation approach has become a powerful tool that can provide quantitative information concerning the dynamic processes at individual particle level (Deng et al., 2013; Zhu et al., 2008). It has been widely used to investigate the mixing process of non-cohesive and cohesive particles (Fan et al., 2018; Figueroa et al., 2009; Lemieux et al., 2007), deagglomeration and packing of cohesive fine particles (Deng et al., 2013; Deng and Davé, 2013; Yang et al., 2000), and so on. However, DEM simulations have faced serious computational challenges in modeling adhesive mixing processes due to the prevalence of large number of cohesive fine particles in such mixing processes. In recent years, several preliminary DEM simulations have been reported, which help better understand the adhesive mixing process. For example, DEM simulations were employed to investigate the exchange and redistribution of fine particles amongst different coarse particles (Nguyen et al., 2016; Nguyen et al., 2015b; Yang et al., 2013, 2015). Those results demonstrate that the transfer of fine particles between coarse particles exhibit different patterns, depending on the collision kinetics and particle properties (Nguyen et al., 2016).

Overall, previous DEM simulations regarding adhesive mixing process have focused on certain specific mixing mechanisms, such as adhesion, deagglomeration or exchange and redistribution (Nguyen et al., 2016; Nguyen et al., 2015b; Yang et al., 2013, 2015). However, investigation of an adhesive mixing process with statistically relevant number of coarse particles has not been reported. For example, the majority of previous work uses only one or two coarse particles in simulations, which does not easily allow for the capturing of overall dynamics and examining the time-scale to reach mixing equilibrium. Further, the collision energy distribution depends on coarse particle collisions, and having such few particles makes it difficult to account for different collision angles that could lead to different mixing quality, even when the collision energy is the same. The problem faced by the authors of previous work is excessive simulation times required to simulate conventional mixing processes, preventing investigation of more realistic simulation scenarios. Thus, such efforts could not examine and capture the complex collision dynamics during adhesive mixing process. Another important issue that requires closer examination is the assessment of mixedness. For ordered mixtures, the smallest relevant scale of scrutiny is an individual coarse particle. Mixedness may be then assessed by analyzing the number of fine particles that are attached to coarse particles and computing a relative standard deviation (RSD), capturing the uniformity of fines with respect to coarse particles. However, this approach does not account for unattached fines, the amounts of which can vary as the surface energy, particle size, and processing conditions are varied. Therefore, the normalized average concentration (NAC) of fine particles per coarse particle is defined as a measure of fine particle coating quality, in addition to the RSD. Consequently, special features of this investigation include: use of larger number of coarse particles, use of high-intensity vibrational mixing which is intended to accelerate the mixing dynamics so as to reach equilibrium in realistic amount of time, and using both the NAC and RSD to assess mixing and coating effectiveness. These enhancements are expected to help fulfil the main objective of this study, which is deepening the mechanistic understanding of the overall adhesive mixing process by putting special emphasis on two important and related dynamic processes: fine particle deagglomeration and their subsequent adhesion to coarse particles, along with their dependence on material properties.

2. DEM simulation

2.1. DEM simulation approach

In discrete element method (DEM) simulation, each particle has translational and rotational motion, governed by the following equations.

$$m_i \frac{d\vec{v}_i}{dt} = \vec{F}_i + m_i \vec{g} \tag{1}$$

$$I_i \frac{d\vec{\omega}_i}{dt} = \vec{T}_i \tag{2}$$