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# Numerical simulation on mixing dynamics of flexible filamentous particles in the transverse section of a rotary drum

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#### ABSTRACT

Flexible filamentous particles are a special kind of particles and play a significant role in many industrial processes. The mixing dynamics of flexible filamentous particles in the transverse section of a rotary drum were analyzed numerically in two dimensions. First, a chain model of slender bodies was introduced for particle dynamic studies, and each individual particle as well as each segment of the particle was tracked during the process. Then, the bulk movement of particles in the transverse section of a rotary drum was explored numerically and mixing dynamics of the particles were further investigated with visual representation. To quantify the quality of mixing, the mixing rates were investigated to determine the mixing extent of particles in the rotary drum. Furthermore, the effects of rotational velocity, flight height and filling degree on mixing dynamics were examined in detail. Moreover, the numerical results were compared with experimental data, and reasonable agreements were obtained. The numerical analyses provide valuable insights into the mixing dynamics of flexible filamentous particles.

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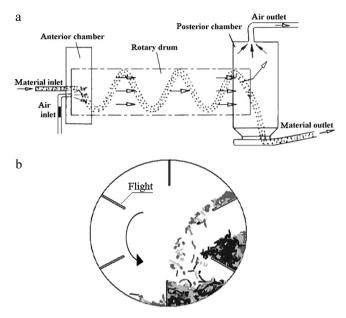
#### 1. Introductions

Many industrial processes involve flexible filamentous particles, such as pulp fibers, pastures, cut-tobacco particles, microfibers in textiles, polymers in medicine, tobacco mosaic virus and DNA molecules in biology (Geng et al., 2011; Jeon & Cox, 2009; Sadlej, Wajnryb, Ekiel-Jezewska, Lamparska, & Kowalewski, 2010; Switzer & Klingenberg, 2004). However, flexible filamentous particles are unique, as they are thin, long, and distinctly different from spherical particles, and the results obtained from spherical particles could not be easily applied to flexible filamentous particles. Fundamental understanding of the behavior of these irregular particles and their particulate systems is still lacking, despite their potentially beneficial impact on many industries. Studies on particle kinematics, particle flows and mixing dynamics could provide useful means to explore particle behavior. In particular, mixing dynamics yield large scale patterns and structures that could provide way to examine particle flows.

At the same time, rotary drums have been extensively employed in chemical, metallurgical, food, tobacco and mineral processing industries, for the purpose of mixing, drying, heating, and chemical reactions. Mixing dynamics in a rotary drum is an important process in particulate industries and is usually accountable for the rate of heat transfer between solids (Geng et al., 2009; Kwapinska, Saage, & Tsotsas, 2006; Van Puyvelde, Young, Wilson, & Schmidt, 1999). This limiting rate factor directly affects the yield and efficiency of the process and the quality of final products, therefore particle mixing is usually a bottleneck for characterizing the bulk movement of particles in the rotary drum (Rajamani, Mishra, Venugopal, & Datta, 2000). Typically, particle properties are important factors, especially the particle shapes (Geng et al., 2009).

Therefore, the aim of this paper is to investigate the mixing dynamics of flexible filamentous particles in a rotary drum, especially in the transverse direction since particle mixing in the transverse direction is a few orders of magnitude faster than that in the axial direction (Geng et al., 2011; Rajamani et al., 2000). In this study, a chain model was used to track individual particles as well as its segments during the mixing process. Moreover, mixing rates were investigated to determine the mixing extent of particles in the rotary drum. Furthermore, the influences of rotational velocity, flight height and filling degree on mixing dynamics of particles were discussed in detail. And the results were compared with that of experimental data available in the literature, thus providing useful information for studying non-spherical particles.

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**Fig. 1.** Schematic diagram of a rotary dryer: (a) longitudinal section plan and (b) transverse section plan.

#### 2. Computational models

#### 2.1. Physical model

The rotary drum studied consists of a long rotating cylindrical shell, which is slightly inclined to allow particles to flow from one end to the other (Lisboa, Vitorino, Delaiba, Finzer, & Barrozo, 2007; Pandey, Song, Kayihan, & Turton, 2006), as shown in Fig. 1(a). Fig. 1(b) shows particle flights through space in transverse section of the drum, which are crucial to particle mixing and drying (Pan, Wang, Yao, & Jin, 2006; Revol, Briens, & Chabagno, 2001; Sheehan, Britton, & Schneider, 2005). Though there are different types of movements, the vertical flights are simple and commonly used in rotary dryers, which were studied as an example in this work due to the complexity of flexible filamentous particles and its simulation technique. Therefore, a two-dimensional model was used to investigate the bulk movement of flexible filamentous particles in the transverse direction of the flighted rotary drum.

#### 2.2. Mathematical model

A chain model for slender bodies was introduced in two dimensions. The following assumptions are introduced (Geng et al., 2009, 2011; Pandey et al., 2006):

- (i) The flexible filamentous particles are long, homogeneous and anisotropic. Each particle consists of three segments, and the segments are treated as rigid slender bodies, which are connected through ball and socket joints. As a result, each particle could be modeled as chains of rigid slender bodies and the particle chain model is presented in two dimensions, as shown in Fig. 2(a). Thus a particle could be treated as a multi-rigid-body system.
- (ii) Equations governing the motion of a model particle are derived from force and torque balances on each segment in the chain, as shown in Fig. 2(b). And Lagrange equations for a multi-rigidbody system are introduced. Meanwhile, additional constraints are imposed on the motion of contacting particles to hold segments together in the chain. The kinetic joints are described

by a set of holonomic algebraic constraints for a constrained multi-body system. Thus the differential equations and the constraint equations for the motion of a multi-rigid-body system can be described as

$$\begin{cases}
\frac{d}{dt} \left[ \frac{\partial T}{\partial \dot{q}} \right] - \frac{\partial T}{\partial \mathbf{q}} = \mathbf{Q} + \mathbf{\Phi}_q^T \lambda + \mathbf{\Phi}_q^{(R)T} \mathbf{F}^{(R)} \\
\mathbf{\Phi}(\mathbf{q}, t) = \mathbf{0} \\
\mathbf{\Phi}^{(R)}(\mathbf{q}, t) = \mathbf{0}
\end{cases} \tag{1}$$

where T is the kinetic energy of the system,  $\mathbf{q}$  is a set of independent coordinates,  $\dot{\mathbf{q}} = d\mathbf{q}/dt$ ,  $\Phi_{\mathbf{q}} = \partial \Phi/\partial q$ ,  $\Phi(\mathbf{q},t) \in R^m$  is the relative distance vector at contact points of the bilateral constraints in consideration of the friction,  $\Phi^{(R)}(\mathbf{q},t) \in R^k$  is the relative distance vector in the tangent direction of the viscous constraint k among the m contact points.  $\mathbf{F}^{(R)}$  is the constraint reacting force in the tangent direction at contact points of the bilateral constraints in consideration of the friction. And  $\lambda$  corresponds to the normal reaction at the contact point.  $\mathbf{Q}$  is the system generalized forces associated with  $\mathbf{q}$ , including gravity, friction and collision force (or collision impulse) during the mixing process. Details of the equations for the two-dimensional chain model were presented in our previous work (Geng et al., 2011).

(iii) Particle-to-particle, particle-to-wall and particle-to-flight collisions are all rigorously modeled.

#### 2.2.1. Collision detection

Each particle and its segments are tracked in order to record the parameters of each segment. This was implemented by using the two endpoints of each segment to decide the particle's position. Parameters such as the distance between two points, coplanar lines, lines in different planes, the distance from a point to a line, etc., were used to decide whether a collision may happen and to detect the collision point if a collision took place.

#### 2.2.2. Collision model

The impulse theorem and the Poisson restriction are implemented for contacts between segments of different particles. If a collision takes place between two particles, it can be treated as a collision between two slender bodies, as shown in Fig. 2(c). If a particle-to-wall collision happens, the wall can be treated as a special particle with heavy mass. The other treatments are the same as that for the segment-to-segment collision. A vertical flight is also assumed as a special slender particle with heavy mass for particle-to-flight collision. Equations governing the motion of each segment have been derived from force and torque balances. Details of collision model can be found in previous work (Geng et al., 2009).

Moreover, periodic boundaries are considered for the mixing process in a rotating drum. The above model has been validated to some extent through simulation and experimental studies in previous work (Geng et al., 2011), focusing on video-imaging analysis to predict particle behavior of flexible filamentous particles in the rotary dryer.

#### 2.3. Mixing extent

Table 1 summarizes the parameters used in simulation (Liu, Specht, & Mellmann, 2005a; McCarthy, Khakhar, & Ottino, 2000). To visualize the effect of initial particle layout in the drum on the particle mixing process by improved Visual Basic codes, three groups of particles with different colors were used and layered in the drum initially with red at the bottom, blue on top and green in between,

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