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GPU-based discrete element simulation on a tote blender for performance improvement

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ABSTRACT

The mixing and flow of granular materials in a conical tote blender are investigated using a GPU-based DEM software to explore new approaches to enhance mixing. The structure and dimensions of the blender and other simulation conditions are set according to experimental data from literature. A parametric study on fill level and rotation rate is carried out from which optimum values are found with respect to mixing rate, productivity and energy consumption. It is also found that the standard horizontal installation of the blender results in poor axial mixing, while inclining the blender at a certain angle can enhance mixing effectively. This may be ascribed to the larger mean particles velocity and better velocity distribution under such conditions, which is confirmed to be a consistent character for relatively large-scale systems. Furthermore, the effect of operating conditions for the inclined blender is also examined. It is close to those for the standard blender but has less effect on mixing rate.

1. Introduction

High quality and fast blending of granular materials is required by many processes in chemical, pharmaceutical and food industries. For many drugs, the active ingredients constitute only a very small fraction of the pill weight, but the effectiveness and safety of the drug is very sensitive to their dose and hence to the homogeneity of their distribution among the pills. The tote blender is one of the most common tumbling blenders widely used in these industries due to its simplicity and reliability [1]. But its wider applications are limited by the slow axial mixing rate. Previous works on tote blenders have focused on their mixing and segregation characteristics [2] and the effect of fundamental parameters [1,3]. Relatively few researches have addressed the ways to enhance their mixing performance.

Computer simulation with discrete element method (DEM [4]) is a promising approach for exploring optimal and new blender designs due to the comprehensive information it can provide for the mixing process, even to the extent that the trajectory and velocity evolution of each particle can be followed. DEM has been found applications in blender studies, such as for rotating drum [5–8], double-cone blender [9], V-blender [3,9–11], tote blender [2,12,13], helical mixer [14,15] and flat blade mixer [16–18]. However, due to computational cost, most simulations still focus on small systems with large particles [19], which restrict the wide application of DEM in the engineering of blenders. In recent years, the emergence of parallel GPU computing seems to offer the possibility of simulating large-scale industrial systems [20], as demonstrated by the present work where the software developed by IPE [21] is employed to study particle mixing in a conical tote blender.

In this paper, we will first investigate the optimal fill level and rotation rate for a 7.5 L blender comprised of a cylindrical bin and a pyramidal hopper sections, and then inclined blenders at different angles in searching for better mixing performance. The tote blender is designed to integrate the functions of blending and transport [13], which can avoid discharging materials into a secondary transport vessel, and then minimize operator contact, hence more and more applications are found in pharmaceutical industry recently. As shown in Fig. 1, the geometry and dimensions of the blender we used are identical to those in the experimental investigation of Ref. [3].

2. Simulation method

With DEM, the motion of each particle can be tracked at every time step. The collision between individual particles can last for some time and occur among several particles based on the time-driven soft-particle method. In our simulation, both translational and rotational motions are considered, as detailed below.

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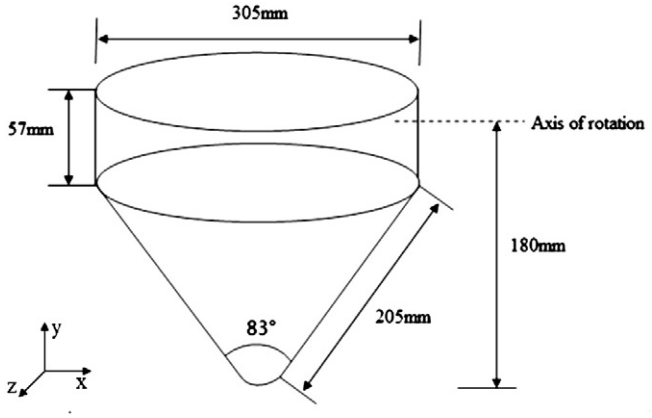

Fig. 1. Dimension of the conical bin-blender used for simulation and experiment [3].

2.1. Model specifications

According to Newton's laws, the equation of motion for the particles is given by

$$m_i \frac{d\boldsymbol{\nu}_i}{dt} = \sum_j \left(\mathbf{F}_{ij}^n + \mathbf{F}_{ij}^t\right) + m_i \mathbf{g} \tag{1}$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_j \left(\mathbf{T}_{ij} + \mathbf{M}_{ij}\right) \tag{2}$$

where $\boldsymbol{\nu}_i$,$\boldsymbol{\omega}_i$,I_i are the translational, angular velocities, and moment of inertial of the particle, respectively. $\mathbf{F}_{ij}^n$,$\mathbf{F}_{ij}^t$ represent the normal and tangential contact forces. $\mathbf{T}_{ij}$ is the torque on particle i caused by tangential force $\mathbf{F}_{ij}^t$ and $\mathbf{M}_{ij}$ is the rolling friction torque.

Many models have been used to describe the contact forces [22], in which Hertz–Mindlin and Deresiewicz models are considered as the theoretically reliable model. However, they are time-consuming especially for a large-scale system due to their complexity. In this work, a simplified model, based on the Hertz, Mindlin and Deresiewicz theories, which was proposed by Zhou et al. [23] is used in our simulations. This model is not only time-affordable but also accurate due to the inclusion of a complete the rolling friction model [24] and consider comprehensive description of the conservative and dissipative forces in both normal and translational motions of the particles. Besides, the accuracy of the flow simulated by this DEM-model has been demonstrated previous researches [11,25]. The values of the simulation parameters for the DEM model in this study, as shown in Table 1, are chosen according to Ref. [3]. The time step chosen for computing should be smaller than a certain critical value to make the algorithm stable and accurate. Tsuji et al. [26] investigated the effect of time step on energy dissipation and found that $\Delta t < \frac{1}{5}\pi\sqrt{\frac{m}{k}}$, which is 1/10 of the natural oscillation period, and hence we have $\Delta t = 10^{-6}$ here.

The simulations are carried out by a GPU-based DEM software (DEMMS V1.0 [21]) running on the Mole-8.5 supercomputer at IPE [27]. In this software, the blender shell is made up of the "frozen" particles, which facilitates the description of complicated geometry though it incurs slightly higher computational cost. The whole simulation system is divided into smaller domains along the x-axis, each processed by one GPU. The cases below 40% filling level were divided into six domains and those above 40% were divided into twelve domains.

Table 1
Simulation parameters for the DEM model.

Properties	Value
Diameter (d)	2 [mm]
Density (ρ)	1500 [kg/m^3]
Young's modulus (E)	2.0 [MPa]
Poisson coefficient (υ)	0.3
Damping coefficient (c_n,c_t)	0.3
Friction coefficient (μ_s)	0.15
Rolling friction coefficient (μ_r) coefficient (μ_r)	0.00025
Time step (Δt)	1×10^{-6} [s]

Table 2
The operating conditions for different cases.

Case	Fill level (%v/v$_{tot}$)	Loading profile	Rotational speed (RPM)
A	35	Left–right	15
B	35	Left–right	45
C	35	Top–bottom	15
D	35	Top–bottom	45

2.2. Statistical methods

The performances of powder blending in the conical tote blender are analyzed both quantitatively and qualitatively. VMD [28], a handy 3D graphic post-processing software originally developed for molecular dynamics simulations, is employed to visualize the mixing process for qualitative analysis. As to quantitative analysis, we evaluate the degree of homogeneity of a mixture and mixing rate by RSD (relative standard deviation) curve and mixing constant.

RSD is a function of the number of blender revolutions (or mixing time). It can be calculated as [29]:

$$RSD = \frac{\sigma}{\overline{\overline{C}}} \tag{3}$$

where

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N}\left(\overline{C}-C_i\right)^2}{N-1}}. \tag{4}$$

In Eqs. (3) and (4), N is the total number of samples and C_i is the concentration of sample i, and $\overline{C}$ is the average concentration of all samples. Besides, the standard deviation for a completely random binary mixture is considered as:

$$RSD_r = \frac{\sigma_r}{\overline{C}} \tag{5}$$

with

$$\sigma_r = \sqrt{\frac{\overline{C}\left(1-\overline{C}\right)}{m}}, \tag{6}$$

where m is the number of particles in a sample. Particle concentration is calculated using a 'boxing-counting' method [2]. By this method, the entire blender domain is divided into cubic domains whose size is chosen as $(10\text{ mm})^3$ in our cases. Each cubic domain with more than 60 particles is considered as a sample for which the numbers of each kind of particles are counted.

To quantify the mixing rate, the mixing constant is employed in our study. According to Ref. [29], the driving force of the mixing process can

Table 3
Sample parameters.

Case	Number of samples	Particles per sample	RSD_r (%)
Simulation	3000	130	8.8
Experiment	–	5500	1.4