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Development of a multi-compartment population balance model for high-shear wet granulation with discrete element method

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ABSTRACT

This paper presents a multi-compartment population balance model for wet granulation coupled with DEM (discrete element method) simulations. Methodologies are developed to extract relevant data from the DEM simulations to inform the population balance model. First, compartmental residence times are calculated for the population balance model from DEM. Then, a suitable collision kernel is chosen for the population balance model based on particle–particle collision frequencies extracted from DEM. It is found that the population balance model is able to predict the trends exhibited by the experimental size and porosity distributions by utilising the information provided by the DEM simulations.

1. Introduction

Wet granulation is a manufacturing process to produce granules with desired properties from small particles and binders, using equipments such as high-shear mixers, rotating drums and fluidised beds. Models for granulation can be broadly separated into particle level models and models which simulate the process at the unit operation level (Michaels, 2003; Heinrich et al., 2015). Models at the particle level are developed to predict inter-particle forces using fundamental physics and Iveson et al. (2001) did an excellent review on such models. At the other end of the scale, models at the unit operation level are used to predict the overall behaviour of granulation processes and this paper focuses on this aspect. Modelling approaches for wet granulation processes at the unit operation level can be loosely separated into two categories: population balance modelling and discrete element method (DEM).

The population balance approach tracks the change in the particle population with time through birth and death processes: for applications in granulation, these processes are usually the coalescence and breakage of particles (Braumann et al., 2007). Traditionally, population balance models are one-dimensional with particle size as the focus. However, one-dimensional models are insufficient to describe granulation processes accurately (Iveson, 2002). Hence, over the last decade, population balance models published in the literature have been at least two-dimensional with liquid and solid concentrations as the properties included (Oullion et al., 2009; Marshall et al., 2013; Barrasso and Ramachandran, 2014) and some models also include particle pore volume (Chaudhury et al., 2014; Darelius et al., 2006; Poon et al., 2008). The main advantage of the population balance approach is that it is capable at considering detailed physical models for processes such as coalescence (Chaudhury et al., 2014; Darelius et al., 2006; Liu and Litster, 2002; Marshall et al., 2013), nucleation (Poon et al., 2008; Oullion et al., 2009) and breakage (Ramachandran et al., 2009). Population balance modelling is also suitable for long time scale studies because of its low computational effort, but it requires certain knowledge of the system in order to include the appropriate processes.

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In DEM simulations, the motion of each particle is computed simultaneously using Newtonian equations of motion (Cameron et al., 2005). It is pointed out by Michaels (2003) that models at the unit operation level often neglect the flow heterogeneity of powder mixing processes and the DEM approach seems to be the ideal solution to bridge this gap. However, DEM is computationally expensive and it does not consider aggregation of granules and other processes such as solidification of granules (Barrasso and Ramachandran, 2014).

Nonetheless, it is possible to include particle flow in population balance models. This is done by dividing the simulation domain into multiple compartments with each of them having its own population balance equation. Thus, each compartment is considered to be perfectly mixed but the process rates can differ between the compartments. A main drawback of this approach is that the flux rates between the compartments are unknown but these can be determined by coupling DEM to population balance models. Population balance models that involve DEM simulations generally fall into three categories: models that use post-processed flux rates from preliminary DEM simulations (Freireich et al., 2011; Bouffard et al., 2012; Li et al., 2012; Sen and Ramachandran, 2013; Chaudhury et al., 2015), models that utilise DEM to develop appropriate aggregation kernels (Gantt et al., 2006; Tan et al., 2004), and models that are directly coupled with DEM (Barrasso et al., 2014, 2015; Barrasso and Ramachandran, 2014). The work carried out in this paper falls into the first two categories.

The main purpose of this paper is to improve an existing multi-compartment population balance model for a batch ploughshare mixer (Lee et al., 2015a,b) with post-processed information from DEM simulations. Previously, the residence times of the compartments were unknown and they were tuned to fit an experimentally measured size distribution. Besides that, the existing model uses a size independent collision kernel and it is found that it is inappropriate for granulation systems (Gantt et al., 2006). In this paper, DEM simulations are performed to determine the appropriate residence times for the compartments and also to implement a size dependent collision kernel.

This paper is organised as follows: A brief description of the population balance model is given in Section 2. Then, Section 3 outlines the DEM simulations carried out in this work. Section 4 describes the stochastic particle method used to solve the population balance model, in particular the adaptation of the majorant technique (Menz et al., 2013; Patterson et al., 2011; Goodson and Kraft, 2002; Eibeck and Wagner, 2000) to accelerate the simulation of collision events. Finally, the ability of the population balance model to predict a set of experimental results is assessed in Section 5.

2. Multi-compartment population balance model

The experimental system considered in this work is the wet granulation of lactose powder with deionised water carried out in a ploughshare mixer depicted in Fig. 1 and it is fully described by Kastner et al. (2013). It is modelled as a series of well-mixed continuous-stirred tank reactors (CSTRs) to account for spatial inhomogeneity and each reactor in the network is given a characteristic residence time, τ. The configuration of the compartmental model is shown in Fig. 2. As previous studies showed that radial dispersion is significantly quicker compared to axial dispersion (Broadbent et al., 1995; Jones and Bridgwater, 1998; Jones et al., 2007), the mixer is compartmentalised in the axial direction in the model. The multi-compartment population balance model was developed by Lee et al. (2015a,b), but the residence times of the compartments were not known and the values were tuned to fit an experimentally measured particle size distribution. In this work, the residence times of the compartments are determined using DEM and the methodology is presented in Section 3.1.

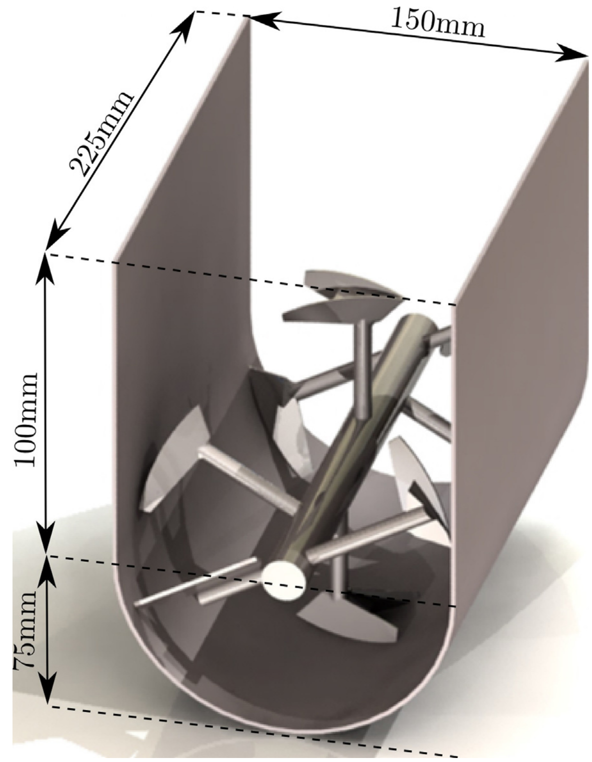

Fig. 1. CAD drawing of the mixer. The radial direction refers to direction in which the blades rotate and the axial direction refers to the direction along the shaft.

In the model, particles take positions in a domain of compartments, $\mathbb{Z} = \{z_1, z_2, z_3\}$. Throughout this work, the residence times of z_1, z_2, and z_3 are denoted as τ_1, τ_2, and τ_3 respectively. In order to capture the spreading of binder liquid which is often regarded as a crucial stage in granulation processes (Faure et al., 2001; Iveson et al., 2001; Reynolds et al., 2004), the middle compartment z_2 is defined as the spray zone where liquid addition occurs. With the exception of liquid addition, each compartment simulates the same particle processes described in Section 2.2, but at different rates to capture the spatial inhomogeneity of the process.

2.1. Type-space

The type-space is the mathematical description of a particle. In this model, the type-space $\mathbb{X} = \{s_o, \ s_r, \ l_e, \ l_i, \ p\}$ has five independent non-negative variables which describe a granule. They are original solid volume s_o, reacted solid volume s_r, external liquid volume l_e, internal liquid volume l_i, and pore volume p.

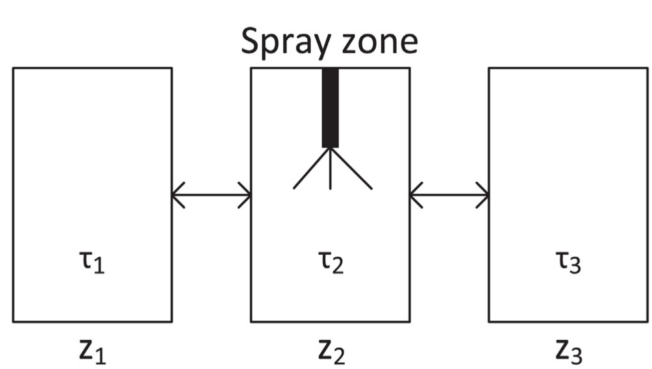

Fig. 2. Configuration of the compartmental model. The mixer (Fig. 1) is compartmentalised in the axial direction. Each compartment has the same size.