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A *priori* prediction of aggregation efficiency and rate constant for fluidized bed melt granulation

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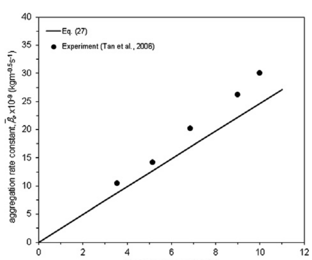
HIGHLIGHTS

- New models for FBMG aggregation efficiency and rate constant have been derived.
- The models are particularly useful for application in population balance equations.
- The models predictions have been compared with experimental data.

GRAPHICAL ABSTRACT



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ABSTRACT

This paper presents a predictive aggregation rate model for spray fluidized bed melt granulation. The aggregation rate constant was derived from probability analysis of particle–droplet contact combined with time scale analysis of droplet solidification and granule–granule collision rates. The latter was obtained using the principles of kinetic theory of granular flow (KTGF). The predicted aggregation rate constants were validated by comparison with reported experimental data for a range of binder spray rate, binder droplet size and operating granulator temperature. The developed model is particularly useful for predicting particle size distributions and growth using population balance equations (PBEs).

1. Introduction

It is widely accepted that the engineering of particulate processes is substantially less well understood than that of fluids. Two difficulties are frequently encountered: the flow of solids is generally much more complex than that of fluids and particles can interact changing their sizes and shapes at almost any point in a process. As a consequence fully-predictive models of fluidized bed melt granulation (FBMG) are very rare.

In FBMG molten binder is sprayed onto a bed of suspended particles. The frequent particle–particle collisions lead to bonding by solidification of the liquid bridges formed between the individual particles. Since the molten binder enters at a point and is then distributed around the bed, these processes are necessarily spatially inhomogeneous. The most widely used model for predicting the particle size distribution (PSD) and growth during granulation, namely, the population balance equation (PBE), adopts a lumping approach, with part of the aggregation rate kernel derived from experiment. An active spray zone (see Fig. 1) is

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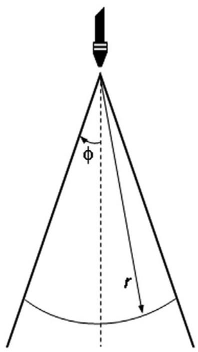

Fig. 1. Schematic representation of the spray zone in a fluidized bed spray melt granulator.

proposed in this paper to derive a purely theoretical model for predicting aggregation efficiency and aggregation rate constant, taking into consideration the spatially distributed processes.

2. Theory

The central assumption in a PBE model is that the aggregation occurs as a consequence of binary particle collisions. By analogy to second order reactions, the rate for this process is given by

$$r_{agg} = \beta_{1,2} N_1 N_2 \tag{1}$$

where r_{agg} is the rate in units of [m^{-3} s^{-1}], $\beta_{1,2}$ is the aggregation kernel for collisions between particles in size classes 1 and 2 in unit of [m^{3}s^{-1}], N_1 and N_2 are the numbers of particles per unit volume [#m^{-3}].

Hounslow and Ryall (1988) has shown that $\beta_{1,2}$ for FBMG can be decomposed into a size dependence component and an aggregation rate constant (β_0) such that,

$$\beta_{1,2} = \beta_0 (D_1 + D_2)^2 \sqrt{\frac{1}{D_1^3} + \frac{1}{D_2^3}} \tag{2}$$

where D_1 and D_2 are the particle sizes of classes 1 and 2. The rate constant, β_0, can be obtained by fitting the PBE predictions of PSD to the experimental data. Combining Eqs. (1) and (2) gives the aggregation rate as follows:

$$r_{agg} = \beta_0 (D_1 + D_2)^2 \sqrt{\frac{1}{D_1^3} + \frac{1}{D_2^3}} (N_1 N_2) \tag{3}$$

In order to develop a theoretically based aggregation rate constant, Tan et al. (2004) derived an expression for β_0 by linking Eq. (3) with the collision rate obtained from the principles of kinetic theory of granular flow (KTGF), to give

$$\beta_0 = \psi g_o \sqrt{\frac{3\theta_s}{\rho_s}} \tag{4}$$

where ψ is a parameter representing the aggregation efficiency, θ_s and g_o represent the mixture granular temperature and the radial distribution function respectively. The latter, g_o, is a function of the solid concentration. According to Tan et al. (2004), θ_s and g_o can both be obtained from suitable models, such as that based on the KTGF, while ψ can be determined experimentally by fitting the measured particles size distribution into a PBE.

In a previous series of studies we discussed the time scale for four microscopic events that contribute to the overall aggregation efficiency of the process. The theoretical models predicting the time scales of (i) granule–granule collision (Chua et al., 2011a), (ii) binder droplet spreading (Chua et al., 2011b) and (iii) droplet solidification (Chua et al., 2011c) have been developed. A graphical summary of the ranges of these time scales have been presented in Chua et al. (2011a). In this paper, we make use of these models to demonstrate that such a theoretical approach can be further extended to predict the granulation efficiency (ψ) and aggregation rate constant (β_0), two of the most important parameters for predicting particle size growth and distribution using the population balance equation.

2.1. Aggregation rate

In this analysis we are interested in expressing the aggregation rate in terms of mass instead of volume, i.e. per kg not m^3 of bed, since reference to volume of the bed has little meaning—neither the actual volume of the bed, nor that of the region where aggregation occurs. Therefore, we write the mass based rate summed over the whole fluidized bed as

$$\bar{r}_{agg} = M_s \frac{d\overline{N}_T}{dt} = -\frac{1}{2} \int \psi r_{coll} \, dV \tag{5}$$

where M_s is the total mass in the bed, $\overline{N}_T$ is the number concentration per unit mass, ψ is the aggregation efficiency, $\bar{r}_{coll}$ is the rate of granule–granule collision per unit volume and V is the volume where aggregation takes place.

Various functions for predicting the collision rate have been reported in the literature (e.g. Kapur and Fuerstenau, 1969; Goldschmidt, 2001; Darelius et al., 2005). Goldschmidt (2001) has shown that, within the context of a two-fluid model, the number of collisions between particles of phases 1 and 2 per unit volume per unit time can be given by

$$r_{coll} = C_{1,2} N_1 N_2 \tag{6}$$

where the collision rate constant is given by

$$C_{1,2} = \pi D_{1,2}^3 g_{1,2} \left[\frac{4}{D_{1,2}} \left(\frac{\theta_s}{\pi} \frac{m_1 + m_2}{2 m_1 m_2} \right)^{1/2} - \frac{2}{3} (\nabla \overline{u}_s) \right] \tag{7}$$

Following Tan et al. (2004), neglecting the divergence of the particle velocity field and assuming that all the particles are of equal density, Eqs. (6) and (7) can be combined to give

$$r_{coll} = g_{1,2} \sqrt{\frac{3\theta_s}{\rho_s}} (D_1 + D_2)^2 \sqrt{\frac{1}{D_1^3} + \frac{1}{D_2^3}} (N_1 N_2) \tag{8}$$

Note that in Eq. (8) we are assuming that $2D_{1,2} = (D_1 + D_2)$, where $D_{1,2}$ is the separation distance between two colliding particles D_1 and D_2 (centre to centre). Substituting Eq. (8) into Eq. (5) after replacing the volume-based number, N, by the mass-based number, $\overline{N}$ (i.e. $N = \overline{N} \rho_s \varepsilon_s$), gives

$$\bar{r}_{agg} = M_s \frac{d\overline{N_T}}{dt} = -\frac{1}{2} \int \psi g_{1,2} \rho_s^2 (\varepsilon_{s,1} \varepsilon_{s,2}) \sqrt{\frac{3\theta_s}{\rho_s}} (D_1 + D_2)^2 \sqrt{\left(\frac{1}{D_1^3} + \frac{1}{D_2^3} \right)} (\overline{N}_1 \overline{N}_2) dV \tag{9}$$

2.2. Granulation efficiency

2.2.1. Probability of wetting

We start by assuming that the drops do not overlap and that the wetted area per particle is equal to a droplet cross-sectional area multiplied by a constant. It follows that for a particle with n drops attached to its surface the probability that a contact point is wet is given by

$$P_w = n \left(\frac{k_w d_o}{D} \right)^2 \tag{10}$$

where d_o and D are the initial droplet and particle diameters. k_w is a constant relating the initial droplet diameter to the final diameter after spreading. In Chua et al. (2011b), we have shown