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Population balance modeling for the growth of agglomerates via primary and secondary agglomeration in gas-fluidized beds

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ABSTRACT

A population balance model is developed for the growth of pre-formed agglomerates in a fluidized bed with several agglomeration mechanisms considered. Primary agglomeration takes place when dry particles collide with the wet surface of the original agglomerate. Secondary agglomeration occurs either by wet particles colliding with the dry surface of agglomerates, or by liquid migration to the top layer of an agglomerate and subsequent collisions with dry particles. The properties of the liquid binder determine the dominant mechanism. The new agglomeration model for high- and low-viscosity liquid binders is implemented in ANSYS FLUENT commercial software. Model predictions agree reasonably well with available experimental results without altering the previously published parameters of the sub-models employed. It is found that the viscosity of the liquid binder and surface asperities play notable roles in the agglomeration. Surface asperities are especially important when asperity heights are of the same order as the thickness of the liquid film.

1. Introduction

Wet granulation in a fluidized bed is generally used as a size enlargement process that occurs due to the successful coalescence of colliding particles. Granulation consists of three phenomena: (a) nucleation, (b) growth and (c) breakage [1]. Although these three phenomena occur simultaneously, there can be circumstances where one dominates over the others. Wet granulation is important in many industrial process, e.g., oil and gas, food, detergents, pharmaceuticals, ceramics and fertilizers. Recently, significant research has been performed addressing both the fundamental, as well as applied, aspects of wet granulation. Several general reviews have been published demonstrating substantial interest in wet granulation [1–5]. In spite of the wealth of such studies at both the fundamental and applied levels, there is still no unique way to test each phenomenon separately, e.g. to test aggregation without consolidation and breakage.

While research on fluidized bed granulation dates back to the 1960s [6,7], active use of population balance modeling (PBM) for fluidized beds is relatively new. PBM is a method to describe the distribution of particle sizes through differential equations. PBM makes it possible to predict observable properties of the product, such as the agglomerate size distribution and the rate of aggregation. Many attempts have been made to model fluidized bed agglomeration in terms of PBM. Population balance (PB) equations can be solved by Monte Carlo (MC) methods, methods of moments (MOM) and discrete methods (DM). The MC method usually does not interface easily with standard process simulators, which generally implements a deterministic integration routine. A recent review of different MC methods was provided by Zhao et al. [8]. In the MOM method [9], the PB equation is transferred into a set of equations for moments to track the particle size distribution (PSD). However, interpretation of PSD from MOM is a challenging task. MOM approaches are particularly useful in cases where the PSD is not required directly. In the DM, a finite number of size intervals is considered as a discretization scheme [10–13]. These approaches have a distinctive advantage over other methods as the PSD is computed directly. The main disadvantage of the DM approach is that one needs to pre-define a number of bins, which may be very large. By using the weighted residual methods it is possible to resolve the whole PSD with a smaller number of discretization points, as shown using both the spectral and spectral element versions of these methods [12]. Recently a number of similar methods have been developed for PBM [14–17] for different applications.

Quite often in PBM, a homogeneous mixture of solid particles is considered as a secondary phase. However, depending on the stage of the agglomeration, the size of the particles and agglomerates may

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vary locally and spatially. This can be due to the localized variations in kinetic rate, segregation of the particles, etc. [18]. In 2009, Rajniak et al. [19] solved the PB equations using MOM for the inhomogeneous particle size distribution with spray agglomeration in a Würster coater. They combined computational fluid dynamics (CFD) and the kinetic theory of granular flow (KTGF) [18,20] for gas-solid flow with MOM. Hounslow [13] used the concept of equi-partition of kinetic energy (EKE model) to find an aggregation kernel, which was later used by Goldschmidt [18] and Tan et al. [7] to derive the agglomeration kernel from KTGF. Note that for large variation in the size of the particle, the expression derived from KTGF using EKE may not be appropriate. Larger particles may start to settle in the fluidized bed, possibly resulting in direct collisions (due to differences in mean velocity between smaller and larger particles.) Furthermore, larger particles may undergo a significantly larger number of collisions with smaller particles, resulting in the larger particles remaining suspended in the bed. Hence, the assumption of equi-partition of kinetic energy might not be appropriate.

Earlier researchers have reported simultaneous consolidation and breakage, together with agglomeration, in fluidized beds [1]. In industrial equipment, as well as in model experiments, it is challenging to find a regime where agglomeration is the dominant mechanism of particle size changes. Furthermore, it is impractical to find an operating condition where only agglomeration takes place in the fluidized bed without consolidation and breakage. Nevertheless, some researchers [19,21] have tried to explain experimental findings of granulation in fluidized beds by modeling agglomeration alone. Weber et al. [22–24] performed a number of experiments based on pre-formed cylindrical agglomerates of sand and water, glass beads and water, and coke and motor oil. They analyzed the effect of liquid properties, together with the influence of the amount of liquid, the size of the primary particles and the size of the agglomerates, as well as the fluidized bed process variables. Their use of pre-formed agglomerates has the potential to control consolidation and breakage robustly, providing unique data to assist in the development of a successful agglomeration model. Furthermore, their data enable evaluation of the limiting mechanisms such as viscous- or capillary-dominated agglomeration. However, in the absence of any theoretical modeling, authors have been unable to completely explain their findings. For example, a single layer on the aggregate would cause only 5 to 9% weight gain compared to their finding of 20 to 50% weight gain. Furthermore, they were unable to explain the differences between 20% weight gain in one case and ~50% weight gain in another case. In this study, we investigate by modeling the growth of preformed aggregates in order to explain the experimental findings and their limitations. This work could also help delineate additional experiments that would allow more accurate determination of agglomeration and breakage phenomena.

In this paper, we model a wetting liquid-solid system. In a completely wetting system the de-wetting of the particle is energetically unfavourable. Hence, de-wetting can happen only under an external force. For this type of liquid-solid system, if two wet particles collide, they separate without significantly disturbing their film thicknesses. (The collision time is in the order of milliseconds, whereas the liquid film spreading time is of the order of seconds [25]). Moreover, in the case of very high viscosity with sufficiently large liquid bridge volume, viscous dissipation dominates over the capillary energy requirement. For example, in the case of liquid Mobil 15w30, which has a viscosity of $\mu = 84.75$ mPa·s, surface tension, $\sigma = 27$ mN/m [23] and density 855 kg/m3, the capillary number ($Ca = \mu u_0/\sigma$, where u_0 is the approach velocity that can be assumed to be of order 1 m/s) is about 3, compared to Ca for water as a binder liquid of about 10^{-2}. It appears that for highly viscous liquids, viscous dissipation is important, whereas for low-viscosity binders the capillary force is dominant. Hence, the viscous coalescence criteria derived by Ennis et al. [26] and modified by Darabi et al. [27,28] can be used for primary agglomeration, together with inelastic losses during collision when a high-viscosity binder liquid is present. Once these wet primary particles collide with the dry surface of the agglomerate, they may make a liquid bridge as liquid adheres to the agglomerate dry surface. Even in the case of high liquid viscosity, if the amount of liquid transferred to the primary particle is very small, the contributions from both viscous and capillary effects become important. Hence, in this work for secondary agglomeration, we account for both viscous dissipation and capillary energy, in addition to energy losses due to inelastic collisions, as discussed by Darabi et al. [27,28]. However, for water as the binder liquid, viscous dissipation remains low, irrespective of the amount of liquid. Hence, both viscous dissipation and capillary energy are important in determining coalescence for low-viscosity liquids.

Primary agglomeration is defined as a successful (i.e. coalescence-inducing) collision between a dry primary particle and the wet surface of the agglomerate for both high and low viscosities. Primary agglomeration can form a single layer on top of an agglomerate. We refer to additional deposition or agglomeration as secondary agglomeration. In the case of a low volume content of a highly viscous liquid in the agglomerate, secondary agglomeration may take place between the wet primary particle and a dry surface. The primary particle becomes wet only after an unsuccessful collision (when the primary particle rebounds after colliding with an agglomerate) with a wet surface of the agglomerate, as no additional liquid is available in the fluidized bed. In the case of high volume content of low-viscosity liquid, secondary agglomeration may take place when the new dry surface created by primary agglomeration becomes wet due to capillary migration of liquid from the interior to the new dry surface.

In the present work, our objectives are to develop a population balance model for the growth of pre-defined agglomerates in a fluidized bed that would consider different agglomeration mechanisms and compare model predictions with available experimental data [22,23] to gain further insights into experimental findings. The resulting model is also used to examine the effects of various process parameters and physical properties of materials on the agglomerate growth and to study different mechanisms of secondary agglomeration.

2. Model description

For the simulations performed in this work, ANSYS FLUENT commercial software [29] is used. Mass and momentum balance equations are solved for the gas and solid phases within the Eulerian framework. In addition, for the solid phase a population balance model for aggregation and a transport equation for wet primary particles are solved. For primary agglomeration, we implement the model of Ennis et al. [26] and Darabi et al. [27,28], whereas for secondary aggregation, we propose two different mechanisms depending on the rheology and quantity of binder liquid.

We consider two different approaches for modeling the growth of agglomerates in fluidized beds: (a) homogeneous population balance modeling using an aggregation kernel derived using KTGF, and (b) inhomogeneous population balance modeling considering collision due to relative velocity. Agglomerates are assumed to be significantly larger than a single particle so that they can be assumed to be spherical and their detailed morphology can be simplified. In the model where an aggregation kernel is derived using KTGF, both the agglomerates and primary particles are considered as a single solid phase. In the inhomogeneous modeling, on the other hand, the primary particles and agglomerates are considered as separate phases. In the KTGF model, collisions between the primary particles and agglomerates take place due to fluctuating velocity, modeled based on the kinetic theory of granular flow. In the inhomogeneous model, collisions between the primary particles and agglomerates take place due to the combined effect of the mean and the fluctuating velocities.