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Product design based on discrete particle modeling of a fluidized bed granulator

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ABSTRACT

Fluidized bed agglomeration is a process commonly used to construct powdered food or pharmaceutical products to improve their instant properties. This works analyzes the influence of a wide range of operating parameters (i.e., fluidization air flow rate, temperature, and liquid injection rate) on growth rate, process stability, and product particle structure. Different granulator configurations (i.e., top spray, Wurster coater, spouted bed) are compared using identical process parameters. The impacts of both process variables and granulator geometry on the fluidization regime, the particle and collision dynamics, and the resulting product structure and corresponding properties are studied in detailed simulations using a discrete particle model (DPM) and lab-scale agglomeration experiments with amorphous dextrose syrup (DE21). The combination of numerical and experimental results allows to correlate the kinetics of micro-scale particle interactions and the final product properties (i.e., agglomerate structure and strength). In conclusion, detailed DPM simulations are proven as a valuable tool for knowledge-based product design.

1. Introduction

Size enlargement and structuring processes (i.e., granulation and agglomeration) in fluidized beds play important roles in the pharmaceutical and fine chemical industries as well as in food technology for improving the flowability and the instant properties of solid products. Dust-free and free-flowing particles can be produced in a process with favorable heat and mass transfer conditions. Furthermore, this technology allows formulation of particles with novel functionalities by applying coating layers or encapsulating the active ingredients.

This work is focused on the agglomeration of amorphous water-soluble food powders. For instant food products, quick redispersability is a key requirement that represents a main consumer benefit compared with fine food powders. To achieve good instant characteristics, agglomerate structures with open pores are desirable because they allow quick penetration of water into the particle matrix. The optimal pore size and agglomerate diameter can be calculated depending on the primary particle size and liquid viscosity. The question of which type of agglomeration equipment is best for producing such particles is a typical example of the challenges in identifying process–structure–property relationships.

Several interdependent micro-mechanisms (i.e., particle collisions, wetting, drying, and phase transitions) govern the process dynamics and complicate predictions of the effects of variable operating conditions on such product properties as structure, strength, and re-dissolution behavior. Profound knowledge of these mechanisms is required to understand the influence of individual process parameters on the final product properties.

The discrete element method (DEM) coupled with computational fluid dynamics (CFD) is a suitable approach for modeling particle interactions in fluidized beds. Information on gas and particle velocities, particle rotation and collision dynamics, which are rather complicated to measure in fluidized beds, can be studied in detail using this technique (Fries, Antonyuk, Heinrich, Dopfer, & Palzer, 2013).

The focus of this work is to build a bridge between the kinetic information from small-scale DEM–CFD simulations and the experimentally obtained particle properties to generate a better understanding of the influence of experimental process parameters on the final product properties.

In a combined numerical and experimental study, both operating parameters and granulator geometry were varied to identify their influences on the fluidization regime. The results show that

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simulated particle and collision dynamics allow prediction of the growth rate as well as the structure and strength of agglomerates, which is a great step forward in model-based product design.

1.1. Types of fluidized bed agglomeration equipment

Fluidized beds for agglomeration are classified according to the nozzle position (top-spray, bottom-spray, or tangential injection) and the operating conditions (batch or continuous) (Uhlemann & Mörl, 2000).

Top-spray granulators are used by the food industry for size enlargement of culinary powders, seasonings, beverage powders, and food ingredients (Bouffard, Kaster, & Dumont, 2005; Jinapong, Suphantharika, & Jamnong, 2008; Werner, Jones, Paterson, Archer, & Pearce, 2007). Bottom-spray installations are applied for agglomeration of dairy powders, as an example. The Wurster coater is a common device used in the pharmaceutical industry to coat tablets and smaller particles in the size range of 20–1000 μm (Karlsson, Rasmuson, van Wachem, & Niklasson Björn, 2009; Tang, Wang, Liew, Chan, & Heng, 2008). Another important field of application is the encapsulation of flavors (Uhlemann & Reiß, 2010). A fourth type of fluid bed is known as the rotor system. A rotor plate placed at the bottom of the bed is rotated, and air is fed through an annular gap between the rotor plate and the wall. The rotor granulator represents the combination of a spheronization device and a fluidized bed. The additional horizontal rotating disk provides a homogeneous and well defined spiral particle motion in the process chamber and allows the application of uniform mechanical stress on the product (Dixit & Puthli, 2009; Jäger & Bauer, 1982; Kristensen, Schæfer, & Kleinebudde, 2000). Fine and poly-disperse solids as well as cohesive powders and needle-shaped particles are manufactured and handled in the food, pharmaceutical, and chemical industries. Usually, a homogeneous fluidization regime cannot be established for such materials due to inter-particle forces and varying fluid drag, which is dependent on particle orientation. The spouted bed offers a promising alternative for this purpose (Epstein & Grace, 2011; Gryczka et al., 2008; Jacob, 2009). Spouted bed technology can be applied for coating (Jono, Ichikawa, Miyamoto, & Fukumori, 2000; Kfuri & Freitas, 2005), spray granulation (Borini, Andrade, & Freitas, 2009; Mann, 1983), and agglomeration (Gryczka et al., 2009; Jacob, 2009).

Except for the rotor granulator and the Wurster coater, all the devices are built with a circular cross-section or with a rectangular cross-section of the process chamber (Jacob, 2010). For continuous operation, conical fluidized bed granulators are equipped with an outlet tube in which classification air is used to re-circulate the fine particles. Devices with a rectangular cross-section are usually equipped with an outlet weir at the end opposite to the inlet.

1.2. Product design

Depending on the specific application, rather different product properties may be relevant, including particle stability, texture, appearance and surface structure, instant wetting and dissolution kinetics, aroma encapsulation and controlled release (Palzer, 2009a, 2009b).

Translation of the desired product properties into tailored particle structures and the process conditions required to generate these structures is a current field of research in various food and pharmaceutical applications (Althaus, & Windhab, 2012; Knorr, 1999; Palzer, 2011; Svanberg, Ahrné, Lorén, & Windhab, 2013; Turchiuli, Eloualia, El Mansouri, & Dumoulin, 2005; Volkert, Puaud, Wille, & Knorr, 2012).

In the context of fluidized bed agglomeration processes, this work attempts to close the circle from the influence of the equipment geometry and operation parameters on the particles and collision dynamics inside the granulator to the resulting particle structure and the strength of agglomerates. Detailed DEM–CFD simulations are used to describe the process system on the scale of individual particles. An introduction to the model is presented in Chapter 2. In parallel with simulations, agglomeration experiments were performed using amorphous maltodextrin (Glucidex DE21, supplied by Roquette SA, France) and pure water as a plasticizer. It should be noted that identical equipment geometries were used in both the simulation and the experiments. The agglomerates produced under different process conditions were analyzed via compression tests, as described in Chapter 3.

Clear correlations were found from comparison of kinetic information of particles and collision dynamics from the model with the strength and stiffness of the experimentally produced agglomerates. The results presented in Chapters 4 and 5 confirm the predictive capacity of the model and describe relationships between the specific influence of the process parameters and equipment geometry on the product structure and particle strength. Based on these results, it can be concluded that DPM simulations offer a significant potential for product design and process optimization, as successfully demonstrated for fluidized bed agglomeration in this work.

2. Mathematical model

Each particle i is tracked individually using Newton's second law of motion to describe translation, as given in Eq. (1), in which the right-hand side considers forces such as pressure gradient, fluid drag, gravity, and contact forces resulting from collisions:

$$m_i \frac{d\mathbf{v}_i}{dt} = -V_i \nabla p + \frac{V_i \beta_{\mathrm{g-p}}}{1-\varepsilon}(\mathbf{u}_\mathrm{g} - \mathbf{v}_i) + m_i \mathbf{g} + \mathbf{F}_{\mathrm{contact},i}, \tag{1}$$

A combination of the Ergun equation (1952) for dense regimes (porosity $\varepsilon < 0.8$) and the correlation proposed by Wen and Yu (1966) for more dilute regimes (porosity $\varepsilon \geq 0.8$) is applied to model the inter-phase momentum transfer coefficient $\beta_{\mathrm{g-p}}$. Particle rotation is calculated using Eq. (2), where I_i, ω_i, and $\mathbf{T}_i$ represent the moment of inertia, the angular velocity, and the torque of particle i, respectively.

$$I_i \frac{d\omega_i}{dt} = T_i. \tag{2}$$

Considering the gas phase as a continuum and discretizing the geometry of the apparatus in the mesh cells, the gas flow profile is calculated using the volume-averaged Navier–Stokes equations, Eqs. (3) and (4). Typically, 2–10 particles fit into one mesh cell.

$$\frac{\partial}{\partial t}(\varepsilon \rho_\mathrm{g}) + \nabla \cdot (\varepsilon \rho_\mathrm{g} \mathbf{u}_\mathrm{g}) = 0 \tag{3}$$

$$\frac{\partial}{\partial t}(\varepsilon \rho_\mathrm{g} \mathbf{u}_\mathrm{g}) + \nabla \cdot (\varepsilon \rho_\mathrm{g} \mathbf{u}_\mathrm{g} \mathbf{u}_\mathrm{g}) = -\varepsilon \nabla p_\mathrm{g} - \nabla \cdot (\varepsilon \boldsymbol{\tau}_\mathrm{g}) - \mathbf{S}_\mathrm{p} + \varepsilon \rho_\mathrm{g} \mathbf{g} \tag{4}$$

As described by Hoomans, Kuipers, Mohd Salleh, Stein, and Seville (2001), $\boldsymbol{\tau}_\mathrm{g}$ denotes the gas-phase stress tensor, and the influence of the particle phase on the fluid flow profile is accounted for with the aid of a sink term $\mathbf{S}_\mathrm{p}$ added to the momentum balance. This term contains the inter-phase momentum transfer coefficient $\beta_{\mathrm{g-p}}$ and closes via the two-way coupling. The drag relationship is required because the fluid flow profile around the particles is not fully resolved.

Contact forces are described using a soft-sphere model (Eq. (5)) proposed by Tsuji, Tanaka, and Ishida (1992) and based on the theory developed by Hertz (1881) for normal impact and a no-slip