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Discrete element study of granulation in a spout-fluidized bed

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Abstract

In this work a discrete element model (DEM) is presented for the description of the gas–liquid–solid flow in a spout-fluidized bed including all relevant phenomena for the study of granulation. The model is demonstrated for the case of a granulation process in a flat spout-fluidized bed, containing four different initial particle size distributions. For each of the cases it was found that particle growth affects the mean of the particle size distribution, but not the standard deviation.

The amount of growth differs significantly for each individual particle and depends strongly on the position of the particle with respect to the spout mouth. Particle growth rapidly decreases with increasing distance from the spout mouth.

It was found that the growth rate scales with the projected surface area of the particle.

Two types of growth have been identified in the simulations, 'peak growth' and 'constant growth'.

Peak growth occurs when particles are exposed to droplets over their entire projected surface area. This type of growth rate is very large, while the period over which the growth occurs is very short (< 4 ms), due to the short residence time of the particles in the peak growth region.

Constant growth occurs when only a small fraction of the particle surface is exposed to the droplets, either because of the location of the droplet beam or because other particles are blocking part of its surface. The growth rate for this type of growth is relatively small, but it can be maintained over a longer period than peak growth.

The majority of the growth is caused by constant growth due to the low solids fraction above the spout mouth, which is caused by the large drag forces exerted by the gas phase on the particles in this region.

The smaller particles within a mixture of differently sized particles are slightly more likely to display peak growth, which is due to the larger concentration of these particles near the spout mouth. In the remainder of the bed all particles display similar growth rates per projected surface area.

For the particle size distributions examined in this work, the ones with a larger average particle size display more growth per projected surface area due to longer residence times near the spout mouth. This is probably caused by the higher particle inertia.

Keywords: Granulation; Fluidization; Hydrodynamics; Mathematical modeling; Multiphase flow; Spout-fluidized bed

1. Introduction

A detailed experimental study of granulation in a spout-fluidized bed is hampered by the fact that (non-intrusive) access of the spout channel is difficult. Therefore, computational methods provide a powerful and attractive alternative for laborious experimental studies. The ultimate objective of a modeling study is to consider an industrial system, but due to the enormous variation in the length and time scales continuum models constitute the only feasible option for the simulation of large-scale spout-fluidized bed granulators. To increase the predictive capabilities of these models, more detailed information needs to be obtained from more sophisticated 'learning' models, like the discrete element model (DEM). This type of model has been used successfully to study a number of applications, such as agglomeration in a rotary drum (Mishra et al., 2002), fluidized bed spray granulation (Goldschmidt et al., 2003), high-shear granulation (Gantt and Gatzke, 2005) and granule microstructure formation (Štěpánek and Ansari, 2005). For a review of different modeling techniques in general and the application of DEM to the field of granulation in particular, the interested reader is referred to the excellent review of Cameron et al. (2005).

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The objective of this work is to make a first assessment of the ability of the discrete particle model to study particle growth and to subsequently gain insight into the particle growth mechanisms prevailing in spout-fluidized beds. In this work we study the granulation process in a spout-fluidized bed, where the particle growth takes place through layering, meaning that droplets are added to the particles at a relatively low rate and that they do not act as a binder. Consequently, agglomeration will not be taken into account.

In this work, a learning model to study the spout-fluidized bed spray granulation process will be presented. The model is based on the hard-sphere DEM originally developed by Hoomans et al. (1996) and extended by Link et al. (2004, 2005) for the simulation of spout-fluidized beds. Since the DEM has proved to be very successful in predicting the main features of the different possible operating regimes in spout-fluidized beds, the focus of this work will be on the incorporation of the additional phenomena relevant for the granulation process, i.e., the treatment of the droplets. The extended model has been used to study in detail the particle growth during granulation in a spout-fluidized bed.

2. Governing equations

In the hard sphere discrete element model rigid particles are assumed to interact through binary, instantaneous collisions. Particle–particle collision dynamics are described by collision laws, which account for energy dissipation due to non-ideal particle interaction by means of the empirical coefficients of normal and tangential restitution, and the coefficient of friction. For further details, the interested reader is referred to the work of Hoomans et al. (1996).

The motion of each individual particle present in the system is calculated from the Newtonian equation of motion:

$$m_p \frac{\mathrm{d}\mathbf{v}_p}{\mathrm{d}t} = -V_p \nabla p + \frac{V_p \beta}{\varepsilon_p}(\mathbf{u}_f - \mathbf{v}_p) + m_p \mathbf{g}, \tag{1}$$

where β represents the inter-phase momentum transfer coefficient due to drag. In this work, a drag relation obtained from lattice-Boltzmann simulations (Koch and Hill, 2001) is used:

$$\beta = \frac{18\mu_f \varepsilon_f^2 \varepsilon_p}{d_p^2}\left(F_0(\varepsilon_p) + \frac{1}{2}F_3(\varepsilon_p)Re_p\right), \tag{2}$$

where the particle Reynolds number is given by $Re_p = \varepsilon_f \rho_f |\mathbf{u}_f - \mathbf{v}_p| d_p/\mu_f$ and with:

$$F_0(\varepsilon_p) = \begin{cases} \dfrac{1+3(0.5\varepsilon_p)^{0.5}+\frac{135}{64}\varepsilon_p \ln(\varepsilon_p)+16.14\varepsilon_p}{1+0.681\varepsilon_p-8.48\varepsilon_p^2+8.16\varepsilon_p^3} & \text{if } \varepsilon_p < 0.4, \\ \dfrac{10\varepsilon_p}{\varepsilon_f^3} & \text{if } \varepsilon_p \geqslant 0.4, \end{cases} \tag{3}$$

$$F_3(\varepsilon_p) = 0.0673 + 0.212\varepsilon_p + \frac{0.0232}{\varepsilon_f^5}. \tag{4}$$

The gas phase flow field is computed from the volume-averaged Navier–Stokes equations given by

$$\frac{\partial}{\partial t}(\varepsilon_f \rho_f) + \nabla \cdot (\varepsilon_f \rho_f \mathbf{u}_f) = 0 \tag{5}$$

$$\frac{\partial}{\partial t}(\varepsilon_f \rho_f \mathbf{u}_f) + \nabla \cdot (\varepsilon_f \rho_f \mathbf{u}_f \mathbf{u}_f) = -\varepsilon_f \nabla p - \nabla \cdot (\varepsilon_f \boldsymbol{\tau}_f) - \mathbf{S}_p + \varepsilon_f \rho_f \mathbf{g}, \tag{6}$$

where the viscous stress tensor, $\boldsymbol{\tau}_f$ is assumed to obey the general form for a Newtonian fluid (Bird et al., 1960):

$$\boldsymbol{\tau}_f = -[(\lambda_f - \tfrac{2}{3}\mu_f)(\nabla \cdot \mathbf{u}_f)\mathbf{I} + \mu_f((\nabla \mathbf{u}_f) + (\nabla \mathbf{u}_f)^{\mathrm{T}})]. \tag{7}$$

Two-way coupling is achieved via the sink term, $\mathbf{S}_p$, which is computed from:

$$\mathbf{S}_p = \frac{1}{V_{\text{cell}}} \sum_{\forall i \in \text{cell}} \frac{V_i \beta}{\varepsilon_p}(\mathbf{u}_f - \mathbf{v}_i) D(\mathbf{r} - \mathbf{r}_i). \tag{8}$$

The distribution function, D, distributes the reaction force acting on the gas phase to the velocity nodes in the (staggered) Eulerian grid. Details of the treatment of the inter-phase momentum transfer can be found in the work of Link et al. (2005).

It is noted that the flow in the spout channel is highly turbulent. However, due to the fact that the flow in the spout region is fully dominated by convection, turbulent sub-grid scale velocity fluctuations can be neglected. Furthermore, in the dense regions around the spout, all relevant turbulent velocity fluctuations are dampened by the particles. Moreover, the particles are hardly influenced by turbulent velocity fluctuations due to their high inertia. For these reasons, no turbulence model was incorporated in the DEM.

The droplets are modeled in a similar way, with the following specific assumptions:

- Due to their low volume fraction the droplets are neglected in the calculation of the gas volume fraction.
- Since the droplets are relatively small, they are assumed to move at their terminal velocity with respect to the gas phase. Consequently, the terminal velocity only needs to be calculated once for each droplet and is approximated assuming Stokes flow, i.e., $\mathbf{v}_\infty = \mathbf{u}_f - \mathbf{v}_d = d_d^2(\rho_d - \rho_f)/(18\mu_f)$, leading to a droplet Reynolds number $Re_d = 26$.
- Droplet–droplet interaction is ignored, because of the small size of the droplets and their low volume fraction.
- Since the impact of an individual encounter between a droplet and a particle is small, these encounters are not calculated in the same way as particle–particle interactions. Droplets are periodically probed for overlap with a particle. To minimize the number of times that droplets move through particles, the droplets are not allowed to move over a distance larger than the radius of a particle during the 'droplet time step'.
- The droplets are assumed to have zero angular velocity.

The mechanism for particle growth is assumed to solely consist of the one-by-one mergers of a droplet with a particle, which leads to the following assumptions. When overlap is detected, the mass and momentum of the droplet are immediately added