DEM-CFD MODELLING OF A FLUIDIZED BED SPRAY GRANULATOR

Lennart Fries∗ Sergiy Antonyuk, Stefan Heinrich† Stefan Palzer‡

∗Hamburg University of Technology, lennart.fries@tuhh.de
†Hamburg University of Technology
‡Nestlé Research Center Lausanne
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DEM-CFD MODELLING OF A FLUIDIZED BED SPRAY GRANULATOR

Lennart Fries, Sergiy Antonyuk, Stefan Heinrich¹ and Stefan Palzer²

¹ Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology
Denickestrasse 15
21073 Hamburg, Germany
T:+49-40-42878 2143; F:+49-40-42878-2678; E: lennart.fries@tuhh.de

² Nestlé Research Center Vers-Chez-Les-Blanc,
Department of Food Science and Technology
Route du Jorat 57
1000 Lausanne 26, Switzerland

ABSTRACT

Coupled DEM-CFD simulations have been performed to study the hydrodynamics of a Wurster granulator on the scale of individual particles. Based on extensive material tests, the collision behaviour of dry γ-Al₂O₃ particles is identified and incorporated into the model. The effect of process parameters like air flow rate and geometry details like the Wurster position is studied. Based on a physical description of the material properties, an effective tool for design and scale-up of a Wurster granulator is obtained.

INTRODUCTION

Fluidized bed spray granulation plays an important role in the manufacturing of powder granules in the food and pharmaceutical industries as it allows producing dust-free and free-flowing particles. Liquid binder is sprayed into a bed of solids to achieve granule growth. Looking on the micro-scale, after the impact of droplets on granules or primary particles and wetting of the particles' surface, drying of the binder layer and evaporation of the solvent initiates layer-wise binder deposition (coating). The Wurster is a common technique in the pharmaceutical industry used to coat tablets. A cylindrical draft tube is inserted vertically into the granulator, as shown in Fig. 1. Combined with a bottom-spray injection nozzle, the Wurster geometry induces a circulating movement of the particles and divides the geometry into two zones. In the central part inside the Wurster tube the particles are transported upwards in a spout. The particles decelerate in the expansion chamber and fall down to the dense region of particles outside the tube, while they are dried by the warm fluidization air. From the dense region, the particles are transported back into the Wurster tube and the circulating motion in the bed is repeated.
The Wurster process is controlled by many parameters which can influence the quality of the coating layer. Although operating conditions and the equipment geometry have been developed through experiments and experience of the process, the actual influence of the fundamental mechanisms in the process is not well understood. The drying rate, and hence the film formation, is highly dependent on the flow field of the gas and particle phases in the equipment.

**MATHEMATICAL MODEL**

Following the concept of the kinetic theory of granular flow (KTGF), multiphase CFD models have been established to describe the fluid dynamics of spout fluidized bed systems [1], [2]. The method allows simulating a lab-scale fluidized bed on a PC workstation within a reasonable period of time. Yet, the method fundamentally lacks a description of the particle-particle interactions. Energy dissipation through non-ideal elastic collisions can only be incorporated to the model with the help of the coefficient of restitution \( e \).

To be able to model a fluidized bed system on the scale of individual particles, several authors have set up discrete particle models (DPM) [3], [4]. Some attempts have been made to model the fluidized bed spray granulation process with DPM [5], [6], [7]. The concept of this modelling technique is briefly introduced in this section.

**The discrete particle phase**

The motion of each individual particle or droplet \( i \) with mass \( m_i \) and volume \( V_i \) in the system is calculated using Newton’s second law

\[
m_i \frac{dv_i}{dt} = m_i \frac{d^2r_i}{dt^2} = -V_i \nabla p + \frac{V_i \beta}{1 - e} (u - v_i) + m_i g + F_{\text{contact},i} + F_{\text{pp},i}
\]

where \( v_i \) is the velocity and \( r_i \) the position of the element \( i \). The forces on the right hand side of Eq. (1) are respectively due to the pressure gradient, drag, gravity, contact forces (i.e. due to collisions) and other particle-particle interactions (for instance Van-der-Waals forces).

The interphase momentum transfer coefficient \( \beta \) is modelled by combining the Ergun (1952) equation for dense regimes \((e < 0.8)\) and the correlation proposed by Wen&Yu (1966) for the more dilute regimes \((e > 0.8)\).
The continuous gas phase

The gas phase is considered as continuum (Euler-Lagrange approach). The geometry of the apparatus is discretized in mesh cells and the motion of the gas phase is calculated using volume-averaged Navier-Stokes equations.

\[
\frac{\partial}{\partial t} (\rho_g u_g) + \nabla (\rho_g u_g u_g) = 0
\]

(2)

\[
\frac{\partial}{\partial t} (\rho_g u_g u_g) + \nabla (\rho_g u_g u_g u_g) = -\varepsilon \nabla p_g - \nabla (\varepsilon \tau_g) - S_p + \rho_g g
\]

(3)

Due to their presence and the volume fraction they require, the particles influence the velocity profile of the gas phase. This effect is accounted for by adding a sink term \( S_p \) to the momentum balance, which contains the interphase momentum transfer coefficient \( \beta \) and closes the two-way-coupling. Forces between the gas and particle phase are of opposite direction and equal magnitude.

Contact model

In case of a collision between two particles, the contact forces are calculated according to a contact model based on the theory developed by Hertz (1882) [8] for the normal impact and a no-slip approximation of the model by Mindlin and Deresiewicz (1953) [9] for the tangential part of the contact force, as proposed by Tsuji [10].

\[
F_{ab,n} = -k_n \cdot \delta_{ab} \cdot n_{ab} - \eta_n v_{ab,n}
\]

(4)

The elastic part of the contact force is represented by a non-linear spring, where the force is proportional to the spring stiffness \( k_n \) and the displacement \( \delta_{ab} \).

Additionally, to account for visco-elastic material properties that cause energy dissipation, a damping factor \( \eta_n \) related to the coefficient of restitution (Tsuji [10]) is included into the model.

The coefficient of restitution \( e \) is defined as the ratio of rebound velocity \( v_r \) to impact velocity \( v \).

\[
e = \sqrt{\frac{E_{kin,R}}{E_{kin}}} = \frac{|v_r|}{v}
\]

(5)

It can be obtained through experiments, as described in the next section.

MATERIALS AND METHODS

Free-fall tests
The impact and rebound behaviour of $\gamma$-Al$_2$O$_3$ granules was analyzed with the help of a free fall test setup as shown in Fig. 2.

Fig. 2: Setup of free-fall tester

The normal coefficient of restitution $e_n$ is independent of the impact velocity $v$ in the investigated range between 0.5 m/s and 5 m/s (Fig. 3, [11]). The experimental values are used to calibrate the contact model in the discrete particle model.

**Coupled DEM-CFD Simulations**

For numerical DPM simulations, a Glatt GF3 insert was modelled. The original geometry was supplied by Glatt Ingenieurtechnik GmbH (Weimar, Germany) and slightly simplified for the simulations, as shown in Fig. 4a. A representation of the mesh used for the fluid dynamics simulations is given in Fig. 4c. The commercial software packages EDEM and Fluent were used to perform simulations with 150,000 spherical particles of a particle diameter $d_p = 2$ mm, which corresponds to a batch size of 0.94 kg at an average particle density of 1500 kg/m$^3$. According to experimental results, the coefficient of restitution was set to 0.8. Air is introduced to the apparatus at the bottom via a segmented distributor plate that consists of three zones. Below the Wurster tube the fluidization air velocity is higher than in the ring-zone due to a larger porosity of the plate.

Additionally, air is injected by a nozzle which is situated at the center inside the Wurster tube. This study focuses on the fluid-dynamic behaviour and does not include the injection of liquid binder.
In a series of case studies, the velocity of the inlet air, the jet injection velocity $u_{\text{spout}}$, the distribution of air between Wurster and annulus and the gap distance $h_{\text{gap}}$ below the Wurster tube was varied. Material parameters were kept constant throughout the simulations as well as the height $h_{W}$ and diameter $d_{W}$ of the Wurster tube. The operating conditions in the case studies are summarized in Table 1.

**Table 1: Overview on the simulation scenarios in this work**

<table>
<thead>
<tr>
<th>Case</th>
<th>$u_{\text{spout}}$ [m/s]</th>
<th>$u_{W}$ [m/s]</th>
<th>$u_{\text{ring}}$ [m/s]</th>
<th>airflow ratio</th>
<th>$h_{\text{gap}}$ [mm]</th>
<th>$h_{W}$ [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>8</td>
<td>4</td>
<td>29.78%</td>
<td>10</td>
<td>200</td>
</tr>
<tr>
<td>2</td>
<td>100</td>
<td>8</td>
<td>4</td>
<td>29.78%</td>
<td>10</td>
<td>200</td>
</tr>
<tr>
<td>3</td>
<td>160</td>
<td>8</td>
<td>3</td>
<td>41.98%</td>
<td>10</td>
<td>200</td>
</tr>
<tr>
<td>4</td>
<td>160</td>
<td>8</td>
<td>3</td>
<td>41.98%</td>
<td>20</td>
<td>200</td>
</tr>
</tbody>
</table>

**SIMULATION RESULTS**

**Influence of gas velocity**

The simulation results show that the velocity of the air injected via the nozzle has a strong influence on the fluid-dynamics of the whole granulator. In Fig. 5, snapshots of the particle positions and their velocities are displayed. The colour indicates the particle velocity magnitude: blue particles move slowly ($v < 0.5$ m/s) and red particles are fast ($v > 1.5$ m/s). Three simulation cases are depicted at the same time step ($t = 1.4$ s).

Visual representations of the simulation results in Fig. 5 and Fig. 8 are taken according to the scheme in Fig. 4b. The central vertical cross section of the apparatus and all parts behind that plane are shown. It can be seen from Fig. 5 that a higher spout velocity causes higher particle velocities inside the Wurster tube. In the acceleration zone near the nozzle, the particles are concentrated to the center of the Wurster for high spout velocities (case 3) whereas they are more evenly distributed over the whole tube for low spout velocities (case 1). The height of the
particle fountain increases with higher spout velocity from 430 mm above the nozzle tip in case 1 to 490 mm in case 3.

![Image of particle fountain and velocity distributions](image)

**Fig. 5:** Instantaneous particle positions and velocity distributions inside the Wurster tube at time $t = 1.4$ s. Colours indicate the velocity magnitude.

To assess the radial distribution of particles in the granulator, horizontal slices were cut out of the simulated geometry. This was done at two different heights, as shown in Figure 4a. The thickness of each of the slices is 10 mm. The first slice is situated in the lower part of the granulator, just below the tip of the injection nozzle. The second slice contains the upper border of the Wurster tube and allows visualizing the flow conditions of particles entering the expansion. Fig. 6 and 7 show instantaneous particle positions in the two slices, seen from the top. Colours indicate the magnitude of the vertical component of the particle velocity. Red particles are transported upwards, blue particles fall down. A comparison can be drawn between the first 3 case studies to evaluate the influence of the spout velocity on the horizontal distribution of the particles.

![Image of horizontal distribution in slice 1](image)

**Fig. 6:** Instantaneous horizontal distribution of particles in slice 1 at time $t = 1.4$ s.

Comparing case 2 and 3 in slice 1 it can be seen that the gas velocity in the outer ring has a strong influence on the bed expansion. For case 3, a dense bed is seen in slice 1 where there is a high porosity in case 2. Looking at the particles inside the Wurster tube it can be observed that the high spout velocity in case 3 tears the particles towards the center of the tube. A comparison between case 1 and 2 in Fig. 6 reveals that at identical flow conditions in the annulus, the gas injection affects the bubble formation in the annulus. At higher spout velocity (case 2) larger bubbles appear.
In slice 2 at the upper end of the Wurster tube, only few particles are present (Fig. 7). Their movement is directed upwards inside the tube and downwards in the annulus at all three cases, indicating that the circulating regime is intact in a wide fluidization range. Along the border of the Wurster tube, a deceleration of the particles can be observed in case 1, whereas at high spout velocity, all particles move faster than 1 m/s at this level (case 3). For low spout velocities as in case 1, some particles are moving downwards at the inside of the Wurster tube, which indicates unwanted back-mixing.

**Influence of the gap distance below the Wurster tube**

The gap distance between the distributor plate and the Wurster tube is a parameter that strongly influences the particle dynamics inside the granulator as it controls the recirculation of particles into the spout. Gaps of 10 mm and 20 mm were compared. It can be seen in Fig. 8 that a larger gap distance below the Wurster increases the number of particles that are transported into the tube. In case 3, in the lower half of the Wurster particles are only present in the center of the tube. All particles rise at a velocity magnitude above 1 m/s which is indicated by green and red colour. Contrary to that, in case 4 particles can be found spread over the whole diameter of the Wurster tube. Near the wall of the tube they move at low velocity, indicated by blue colour.
CONCLUSIONS

Process parameters like the spout velocity and geometrical settings like the Wurster gap height influence the fluid-dynamics of a Wurster granulator, which was analysed with the help of coupled DEM-CFD-simulations. Based on experimental data of the impact behaviour of visco-elastic particles, the fluidization regime and based on that the functionality of a Wurster granulator can be predicted. Future measurements in a real Wurster coater will deliver results to validate the model.

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REFERENCES


KEY WORDS

Fluidized bed spray granulation, discrete element modelling, Wurster coater, CFD, fluid dynamics