Predicting the Performance of Different Fluidized and Spouted Beds for Spray Granulation using CFD-DEM Simulations

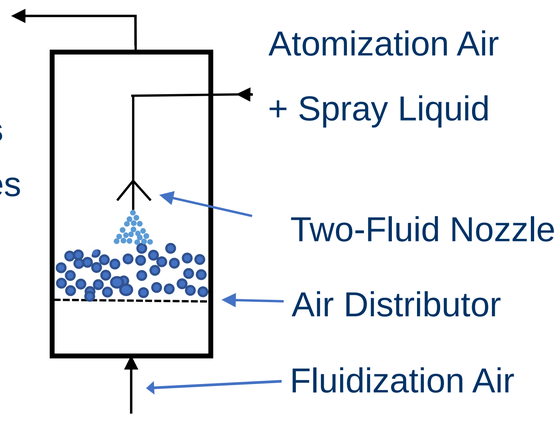
Paul Kieckhefen[1], Moritz Höfert[2], Swantje Pietsch[1], Stefan Heinrich[1]

[1] Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Germany

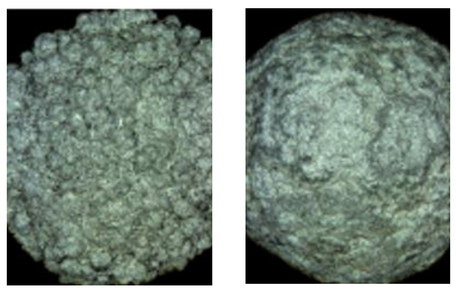
[2] BASF SE, Ludwigshafen am Rhein, Germany

Introduction

- Fluidized beds are excellent apparatuses for the formation of **tailor-made particles**
  - **Granulation**: layered growth of particles by spraying solids-containing liquid
  - **Microprocesses** in droplets and on surface liquid determine **structure** of particle and therefore its properties
- **CFD-DEM simulations** provide detailed insight into hydrodynamic behavior of fluidized beds
  - Evaporation of surface liquid, droplet motion and deposition can be tracked for every particle
  - Track **fate of individual particles**
  - Track properties of droplets and impact parameters
- **Goal:** Predict particle structure from simulations directly

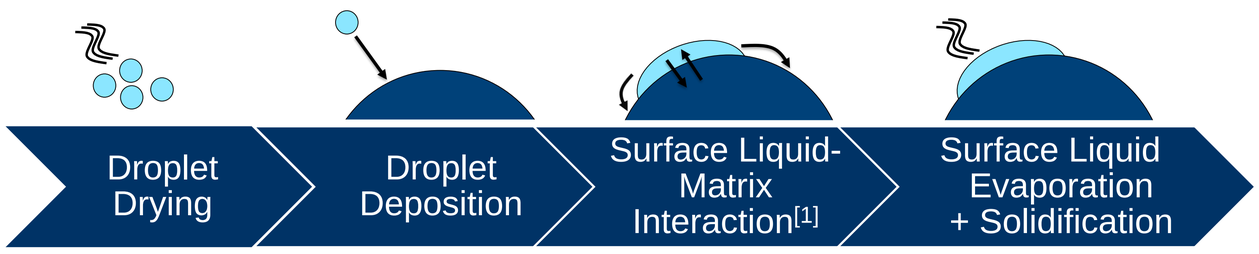


Schematic of a Fluidized Bed Spray Granulation Process



Granulation Products exhibiting Different Surface Structures

Microprocesses in Layering Spray Granulation



- **Nucleation**
- Droplet size
- Rebound / Spreading / Splashing
- **Spreading**
- **Dissolution**
- **Imbibition**
- **Crystallization / Precipitation**

Tracking of **impacted droplet state** and **timescale of drying** can be used as **target variables/tracked quantities** in lieu of resolving surface processes

Workflow for Predicting Product Properties

Prior State of the Art [2,3]

1. Calibration

Process Conditions → Experiment → Product Property

2. Mapping

Process Conditions → Scalar Drying Potential

$$\eta_{\mathrm{drying}} = 1 - \frac{y_{\mathrm{H_2O}}^{\mathrm{wb}} - y_{\mathrm{H_2O}}^{\mathrm{out}}}{y_{\mathrm{H_2O}}^{\mathrm{wb}} - y_{\mathrm{H_2O}}^{\mathrm{in}}}$$

Product Property = f(η_{drying})

3. Prediction

New Process Conditions → Drying Potential → Apply Mapping → Predicted Product Properties

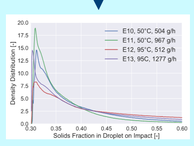
\+ Easy
\+ Usable for salt solutions
\- Unusable for suspensions
\- Restricted to similar geometry

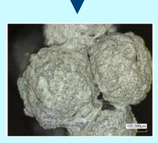
Our Approach

1. Calibration

Process Conditions → Instrumented Simulation / Experiment

Tracked Quantity Distribution





Product Property

2. Mapping Product Property = f(Moments of Tracked Quantity Distribution)

3. Prediction

Different Process Conditions, Geometry → Simulation / Application of Mapping → Predicted Product Properties

\+ Geometry-independent
\+ Usable for salt solutions
\+ Operates on distributions of particles
\+ Usable for suspension
\+ Wider applicability
\- Requires simulations

Our concept uses an indirect approach in relating product properties to quantifiers of the microprocesses to their resulting surface structures and thus particle properties. This allows for

✓ **Prediction of Scale-Up Effects (incl. dissimilar proportions)**
✓ **Diagnostics in Case of Sub-Par Product Quality**

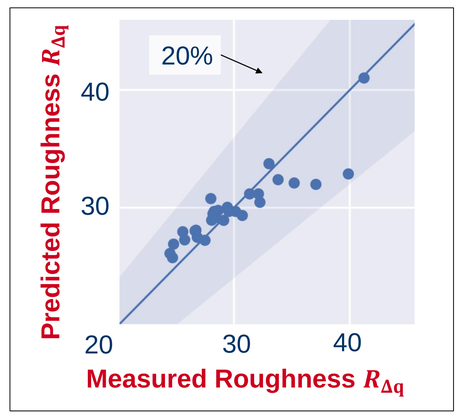
Product Property – Tracked Quantity Mapping

- **Granulation experiments** in GF3 (ø 250 mm) bottom-spray fluidized bed, 31 total experiments
  - Vary spray rate, air temperature, spray air temperature, spray pressure (droplet size)
  - Injection of sodium benzoate (30 wt-%) onto crystalline cellulose particles (d = 650 µm)
- **Surface roughness** characterization using confocal laser-scanning microscope (Keyence)
- Digital twin simulations with same process conditions, tracking
  - Particle liquid layer evaporation time t_{evap}
  - Droplet solution concentration $x_{\mathrm{s,impact}}$
  - Droplet impact velocity v_{impact}
- Perform linear regression between statistical moments μ of tracked quantities in sim. and roughness values $R_{\Delta \mathrm{q}}$ from experiments
  - Dimensionality reduction by L1-regularization

Resulting Mapping: $R_{\Delta \mathrm{q}} = \begin{pmatrix} 0.312 \\ -0.722 \\ -78.4 \\ -0.216 \end{pmatrix} \cdot \begin{pmatrix} \mu_0(t_{\mathrm{evap}}) \\ \mu_2(v_{\mathrm{impact}}) \\ \mu_1(x_{\mathrm{s,impact}}) \\ \mu_2(x_{\mathrm{s,impact}}) \end{pmatrix} + 25.6$

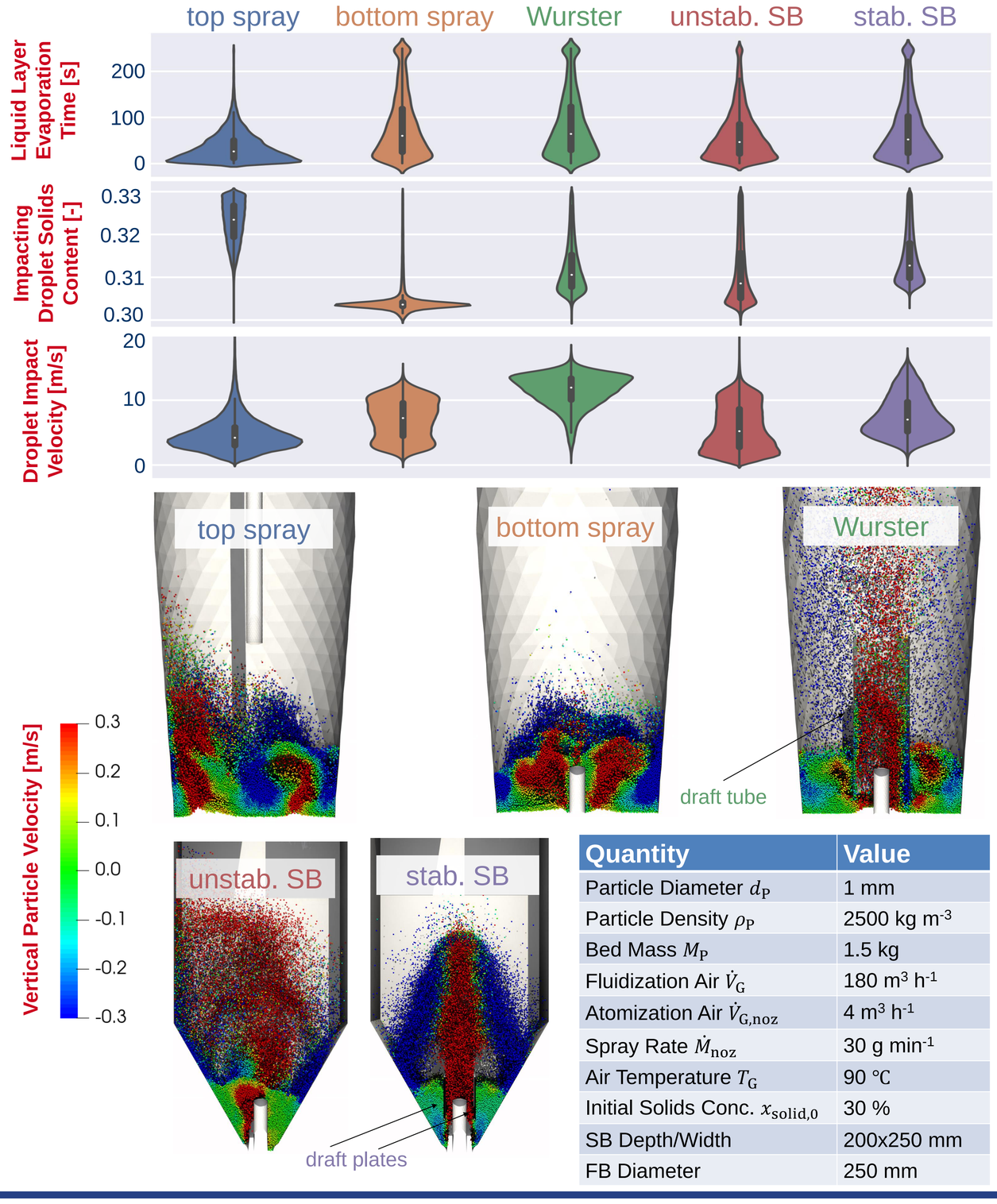
Design of Experiments
↓ Result: Process Conditions
Granulation Experiments
↓ Result: Product Particles
Confocal Laser-Scanning Microscopy
↓ Result: Roughness Value
Map Roughness Values to Tracked Quantities

Experimental Workflow



Parity Plot

Tracked Quantities in Different Granulators



Quantity	Value
Particle Diameter d_{P}	1 mm
Particle Density ρ_{P}	2500 kg m^{-3}
Bed Mass M_{P}	1.5 kg
Fluidization Air $\dot{V}_{\mathrm{G}}$	180 m^3 h^{-1}
Atomization Air $\dot{V}_{\mathrm{G,noz}}$	4 m^3 h^{-1}
Spray Rate $\dot{M}_{\mathrm{noz}}$	30 g min^{-1}
Air Temperature T_{G}	90 °C
Initial Solids Conc. $x_{\mathrm{solid,0}}$	30 %
SB Depth/Width	200x250 mm
FB Diameter	250 mm

Summary

- CFD-DEM provides more information over state-of-the-art design guidelines,
  - uses **distributions** rather than average quantities
  - Advantage: **Geometry-independence**
- Granulator geometries with **identical global drying conditions** yield very **different tracked quantity** distributions
  - Largest influence: Direction of spray
- Next Step: use method for scale-up

Variant	Surface Liquid Drying	Droplet Drying	Droplet Impact Velocity
Stabilizing Internals (draft tube, draft plates)	•	↑	↑
Counter-Current Spray (vs bottom spray)	↑↑↑	↑↑↑	↓↓↓
Spouting (vs bottom spray)	↑	↑↑	↓

References

[1] Heine et al.: *Droplet deposition on amorphous particles in a fluidized bed spray agglomeration process*, Granulation Workshop, Lausanne, (2013).

[2] Schmidt et al.: *Shell porosity in spray fluidized bed coating with suspensions*, Advanced Powder Technology (2017).

[3] Rieck et al.: *Influence of drying conditions on layer porosity in fluidized bed spray granulation*, Powder Technology (2015).