Predicting Product Properties of Fluidized Bed Spray Granulation using CFD-DEM Simulations

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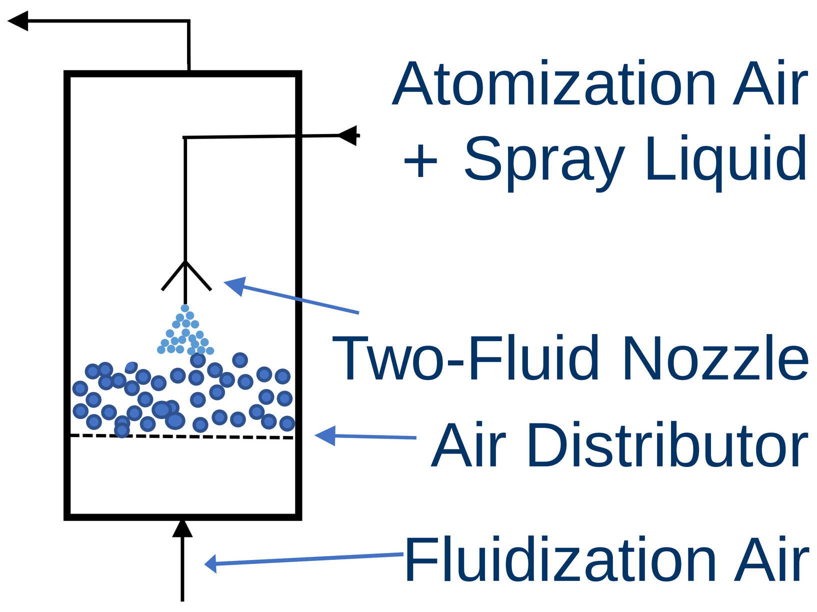
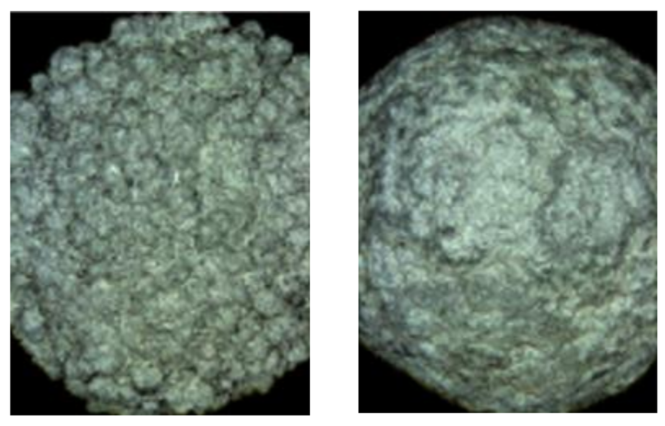
Introduction

- Fluidized beds are excellent apparatuses for the formation of **tailor-made particles**
  - **Granulation**: growing particles by spraying coating with 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 single particle**
  - Track properties of droplets and impact parameters
- **Goal:** Predict particle structure from simulations directly



Schematic of a Fluidized Bed Spray Granulation Process



Example Granulation Products exhibiting Different Surface Structures

Workflow for Predicting Product Properties

Prior State of the Art [4,5]

1. Experiments

2. One-dimensional Correlation of **Macroscopic Drying Potential** to Shell Porosity

$$\eta_{\text{drying}} = 1 - \frac{y^{\text{wb}}_{H_2O} - y^{\text{out}}_{H_2O}}{y^{\text{wb}}_{H_2O} - y^{\text{in}}_{H_2O}}$$

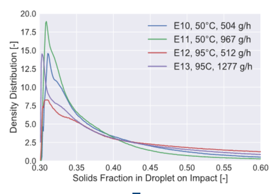
$$\varepsilon_{\text{shell}} = f(\eta_{\text{drying}})$$

3. Apply Correlation to New Process Conditions

Our Approach

1. Calibration

Set of Macroscopic Process Conditions → Instrumented Simulation → Tracked Quantity; → Experiment → Product Property



2. Mapping Product Property and Tracked Quantities

3. Prediction

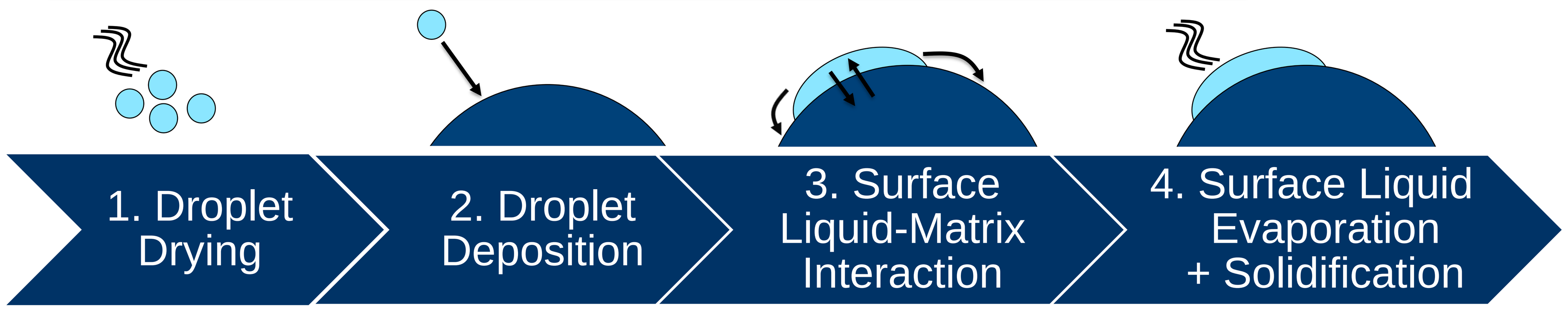
Different Process Conditions, Geometry → Simulation / Application of Mapping → Predicted Product Properties

Our approach 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 Granulator Geometry Influence**
- ✓ **Prediction of Scale-Up Effects (incl. dissimilar proportions)**
- ✓ **Diagnostics of Sub-Par Product Quality**

compared to the state of the art.

Microprocesses in Layering Spray Granulation



- Droplet drying determines **viscosity at impact**
  - Dependent on droplet size, temperature, humidity, rel. velocity
- High viscosities (= concentrations) at impact correlate negatively with dense layering (= high roughness)

- Surface liquid interacts with surface matrix[1]
  - **Spreading** [2]

$$R(t) = \left(\frac{24 V_{\text{drop}} \sigma (\cos(\theta_0) - \cos(\theta_\infty))}{\pi \, \eta}\right) t^{1/4}$$

  - **Dissolution**[3]

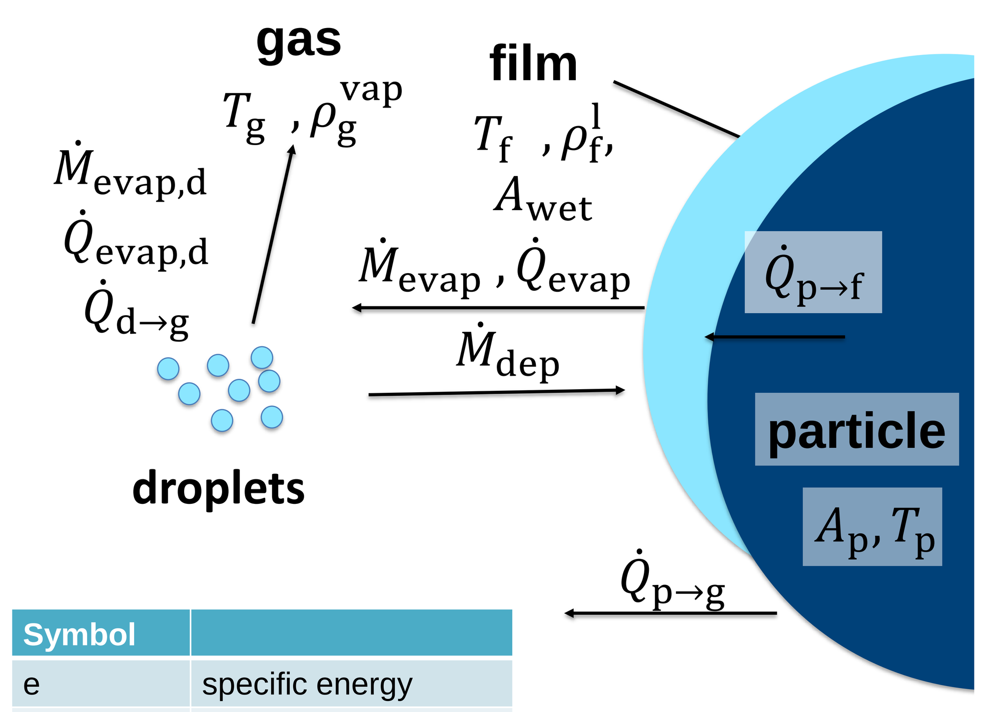
$$\dot{m}_{\text{diss}} = \frac{D A_{\text{layer}}}{h_{\text{layer}}} \left(c^{\text{sat}}_{\text{layer}} - c_{\text{layer}}\right)$$

  - **Imbibition** into pores
- Long event timescales correlate positively with dense layering (= low roughness)

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

Heat and Mass Transfer Modelling in CFD-DEM

- **Balances for film**
  - $\frac{dM_f}{dt} = +\dot{M}_{\text{dep}} - \dot{M}_{\text{evap}}$
  - $\frac{dE_f}{dt} = +\dot{Q}_{\text{dep}} - \dot{Q}_{\text{evap}} - \dot{Q}_{f\to p} - \dot{Q}_{f\to g}$
- **Balances for gas**
  - $\frac{dM_g}{dt} = +\dot{M}_{\text{evap}}$
  - $\frac{dE_g}{dt} = +\dot{Q}_{\text{evap}} + \dot{Q}_{f\to g} + \dot{Q}_{p\to g}$
- **Balances for particle**
  - $\frac{dE_p}{dt} = +\dot{Q}_{f\to p} + \dot{Q}_{p\to g}$
- **Closures**
  - $\dot{M}_{\text{evap}} = \beta A_f \left(\rho^*_f(T_g, \rho_g) - \rho_g\right)$
  - $\dot{Q}_{\text{evap}} = \dot{M}_{\text{evap}} \Delta h_{\text{evap}}$
  - $\dot{Q}_{f\to g} = \alpha_g A_f (T_f - T_g)$
  - $\dot{Q}_{f\to p} = \alpha_{fp} A_f (T_f - T_g)$
  - $\dot{Q}_{p\to g} = \alpha_g (A_p - A_{\text{wet}})(T_p - T_g)$

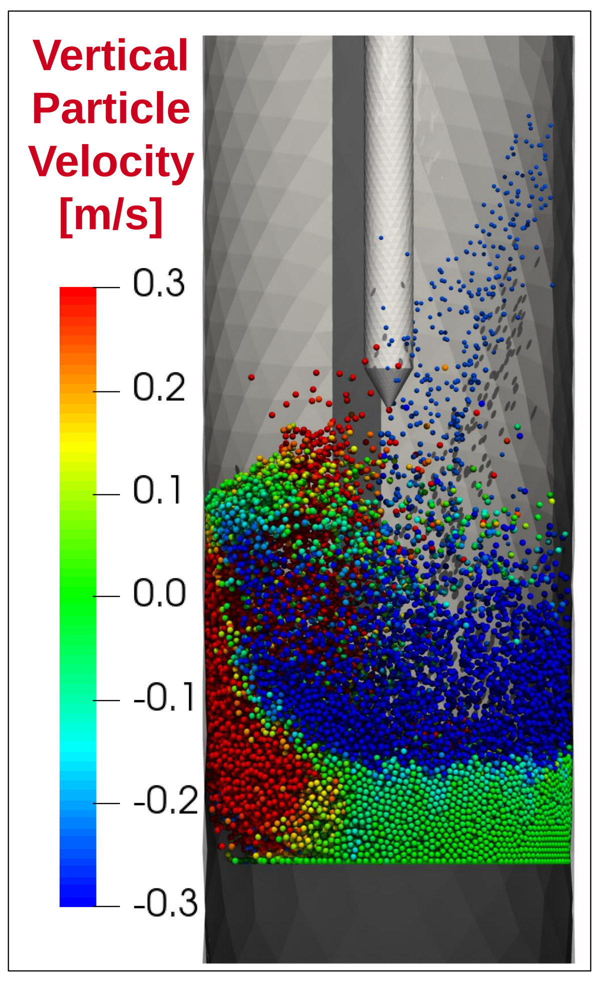


Symbol	
e	specific energy
α	heat transfer coeff.
β	mass transfer coeff.
A	area
M	mass
E	energy
Q	heat
T	temperature

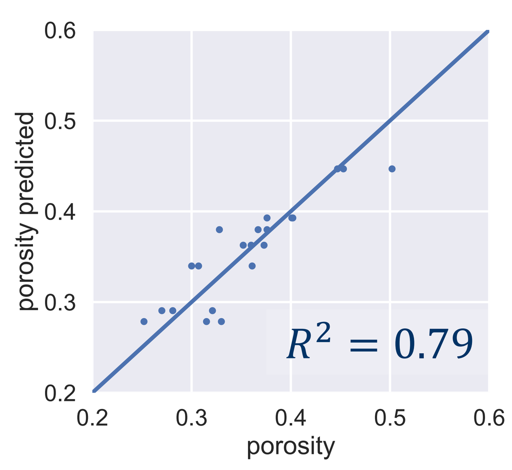
Subscript	
p	particle
f	film
g	gas
dep	deposition

Application: Spray Granulation Case

- Reference experimental case [4] reproduced in simulations
  - Lab-scale (ø 150 mm) top-spray fluidized bed
  - Injection of limestone suspension onto glass particles (d = 650 µm)
  - CT measurement of particle shell porosity
  - Varied spray rate, air temperature $T_{\text{air,in}}$, suspension concentration $x_{\text{susp},in}$, atomization pressure p_{noz}
  - Tracked particle liquid layer **evaporation time** $t_{\text{evap},50}$ and **suspension concentration** x_{susp} in droplets

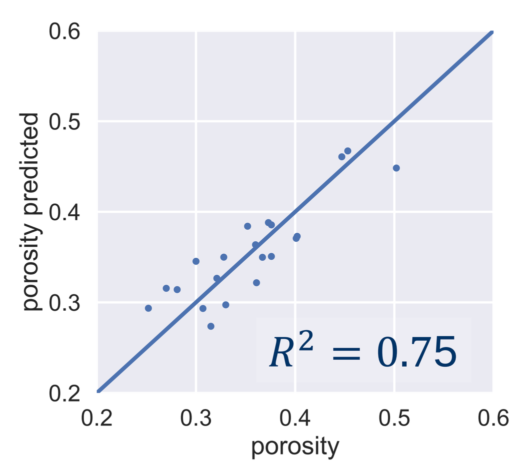


Mapping using Macroscopic Quantities



$$\varepsilon_{\text{shell}} = \begin{pmatrix} 1.1E-3 \\ 7.3E-1 \\ -6.0E-3 \end{pmatrix} \cdot \begin{pmatrix} T_{\text{air,in}} \\ x_{\text{susp,in}} \\ p_{\text{noz}} \end{pmatrix} + 0.24$$

Mapping using Micro-Scale Quantities



$$\varepsilon_{\text{shell}} = \begin{pmatrix} -8.3E-3 \\ -2.3E-1 \\ 6.8E-1 \end{pmatrix} \cdot \begin{pmatrix} t_{\text{evap},50} \\ t_{\text{evap,skew}} \\ x_{\text{susp},50} \end{pmatrix} + 0.68$$

Microscopic tracked quantities predict the product quality with same confidence as macro-scale parameters (process conditions).

References

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

[2] Ogarev et al. : *Spreading of Polydimethylsiloxane Drops on Solid Horizontal Surfaces*, The Journal of Adhesion, (1974).

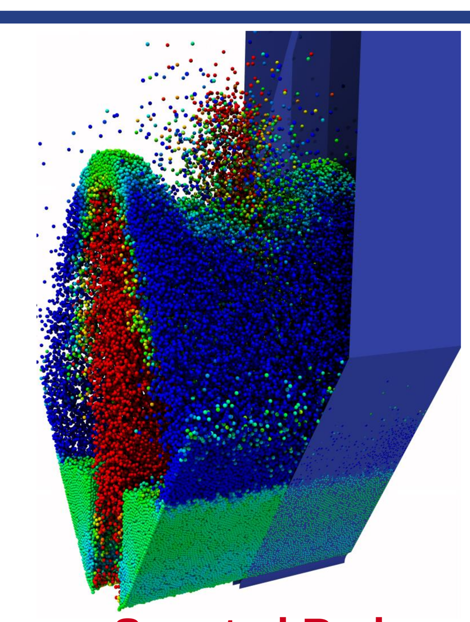
[3] Noyes and Whitney: *The rate of solution of solid substances in their own solutions*, Journal of the American Chemical Society, (1897).

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

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

Next Steps

- Apply method
  - Compare granulators with different geometries
  - Perform **product-driven, simulation-aided scale-up**
- Develop **resolved pore-scale simulations** of drying to close tracked quantity-surface structure gap



Spouted Bed Granulator