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

Microprocesses in Layering Spray Granulation

1. Droplet Drying
2. Droplet Deposition
3. Surface Liquid-Matrix Interaction
4. Surface Liquid Evaporation + Solidification

- 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)

Track 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
  - \[ \frac{d}{dt} \rho_m A_m \eta_m = \frac{\delta_{\text{evap}} - \delta_{\text{cond}}}{\rho_m} (\Delta T_m) \]
- Balances for gas
  - \[ \frac{d}{dt} \rho_{\text{gas}} V_{\text{gas}} \delta_{\text{evap}} = \frac{\delta_{\text{evap}}}{\rho_{\text{gas}}} (\Delta T_m) \]
- Balances for particle
  - \[ \frac{d}{dt} \rho_p V_p \delta_{\text{evap}} = \frac{\delta_{\text{evap}}}{\rho_p} (\Delta T_m) \]

Closures

- \[ \delta_{\text{cond}} = \beta \delta_m (T_r - T_p) \]
- \[ \delta_{\text{evap}} = \delta_m \delta_{\text{evap}} \]
- \[ \delta_{\text{gas}} = \delta_m \delta_{\text{gas}} \]
- \[ \delta_{\text{dep}} = \delta_m \delta_{\text{dep}} \]

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
3. Apply Correlation to New Process Conditions

Our Approach

1. Calibration
2. Mapping Property and Tracked Quantities
3. Prediction

- 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.

Application: Spray Granulation Case

  - 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 \( T_{\text{air}} \), suspension concentration \( x_{\text{susp,In}} \), atomization pressure \( p_{\text{noz}} \)
  - Tracked particle liquid layer evaporation time \( t_{\text{evap,50}} \) and suspension concentration \( x_{\text{susp}} \)

Heat and Mass Transfer Model

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

References


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

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