Benchmarking a Novel 0-D Model Against Data from Two-Fluid Model Simulations of a Wet Fluidized Bed

Stefan Radl, Mohammadsadegh Salehi
Institute of Process and Particle Engineering, Graz University of Technology

Maryam Askarishahi
Research Center Pharmaceutical Engineering GmbH, Graz

radl@tugraz.at
Phenomena governing wet fluidized beds (WFBs)

- Deposition
- Heat exchange
- Evaporative cooling
- Sprayed water
- Deposited droplets
- Evaporation
- Vapor
- Particle

**References**

Askarishahi et al. (2017), AIChE Journal, 63:2569-2587
https://github.com/CFDEMproject

https://www.glatt.com
Motivation

developing a toolset (CFD-DEM/TFM/0D) to predict WFB performance

Euler-Euler-Euler Approach
Two-Fluid Model (CFD-TFM)

Compartment (0D) model

https://mfix.netl.doe.gov
Model implementation mass balance for water (liquid)

\[
\frac{\partial}{\partial t} (\varepsilon_g \rho_g x_{wl}) + \nabla \cdot (\varepsilon_g \rho_g x_{wl} \mathbf{u}_g) = \nabla \cdot (D_g \nabla \varepsilon_g \rho_g x_{wl}) + \dot{S}_{\text{spray}} - \dot{S}_{\text{evap}} - \dot{S}_{\text{depos}}
\]

**Droplet evaporation**

\[
\dot{S}_{\text{evap}} = (\rho_{w,\text{sat}} - \rho_f \mu_{wv}) a_d \beta_d \varepsilon_d
\]

- \(\mu_{wv}\): vapor mass loading
- \(\rho_{w,\text{sat}}\): saturation density
- \(\varepsilon_d\): droplet volume fraction
- \(\beta_d\): mass transfer coeff.
- \(a_d\): specific surface area

**Droplet deposition**

\[
\dot{S}_{\text{depos}} = -\lambda |\mathbf{u}_d - \mathbf{u}_p| \mu_{wli} \varepsilon_g \rho_g
\]

- \(\lambda\): Filtration coefficient after Kolakaluri’s Model
- \(\mu_{wli}\): liquid mass loading
- \(\varepsilon_g\): gas volume fraction

Model implementation mass balance for water vapor

\[
\frac{\partial}{\partial t} (\varepsilon_g \rho_g x_{wv}) + \nabla \cdot (\varepsilon_g \rho_g x_{wv} u_g) = \nabla \cdot (D_{gn} \nabla \varepsilon_g \rho_g x_{wv}) + \dot{S}_{dry} + \dot{S}_{evap}
\]

Accumulation Convection Diffusion/Dispersion Sources

**Particle drying**

\[
\dot{S}_{dry} = (\rho_{w, sat} - \rho_g \mu_{wv}) a_p \psi_{liq} \beta_p \varepsilon_s
\]

\[
\psi_{liq} = 1 - \left[ 1 - f \right] \phi_p / f
\]

\( \mu_{wv} \): vapor mass loading
\( \rho_{w, sat} \): saturation density
\( \phi_d \): droplet volume fraction
\( \beta_p \): mass transfer coeff.
\( a_p \): specific surface area
\( f \): droplet footprint area
\( \phi_p \): coating number

**Kariuki’s Model**

**Continuous film, \( \psi_{liq} = 1 \)**

CFD-TFM

fluidized bed performance assessment
Conical spray zone

\[ d_d = 20\mu m \]
\[ u_d = 7 \, m/s \]

**CFD-TFM simulation**

**Setup and operating parameters**

\[ T_g = 333 \, K \]
\[ u_g = 0.5 \, m/s \]

\[ L_{bed} = 0.23 \, m \]
\[ H_{bed} = 0.75 \, m \]

\[ d_p = 400 \, \mu m \]

https://www.glatt.com
Qualitative performance of WFB

Time: 0 [s]

LoD

ε_g < 0.85
ε_g
ε_g < 0.85
ε_g < 0.98
ε_g
ε_g > 0.9

©MaryamAskaris

©MaryamAskarishahi
CFD-TFM

the degree of uniformity
Uniformity of bed
How to assess?

Is it possible to represent the bed performance with the single values?

Temperature | LoD | vapor content

How uniform is the distribution in the bed?

Qualitative
The time-averaged contour-plots for the exchange rates and the flow properties

Quantitative
The uniformity degree through LoD and temperature standard deviation
Uniformity degree: **Qualitative** examination

Time-averaged flow property distribution

- **droplet mass fraction**
- **bed voidage**
- **vapor mass fraction**

30.10.2018
Uniformity degree: **Qualitative** examination
Time-averaged exchange rate distribution

- **drying rate** $\dot{S}_{\text{dry}} [kg/m^3 s]$
  - $5.3 \times 10^{-3}$
  - $3.5 \times 10^{-3}$
  - $1.8 \times 10^{-3}$
  - $0.0 \times 10^{+00}$

- **evaporation rate** $\dot{S}_{\text{evap}} [kg/m^3 s]$
  - $1.8 \times 10^{-26}$
  - $1.4 \times 10^{-02}$
  - $2.9 \times 10^{-02}$
  - $4.3 \times 10^{-02}$

- **deposition rate** $\dot{S}_{\text{depos}} [kg/m^3 s]$
  - $1.6 \times 10^{-01}$
  - $1.0 \times 10^{-01}$
  - $5.2 \times 10^{-02}$
  - $0.0 \times 10^{+00}$

30.10.2018
CFD-TFM versus 0D model
0D model validity against TFM approach
effect of spray rate

\( \dot{m}_{\text{spray}}^{\text{norm}} \) is defined as the ratio of spray rate to the maximum spray rate (\( RH_{\text{out}} = 100\% \))

- **particle LoD**
- **gas temperature**
- **gas vapor content**
0D model validity against TFM approach
effect of spray rate

Effect of bed aspect ratio

particle LoD

\[ \frac{L_0}{L_{bed}} = 0.65, \text{TFM} \]
\[ \frac{H_0}{L_{bed}} = 0.65, \text{0D} \]
\[ H_0/L_{bed} = 0.15, \text{TFM} \]
\[ H_0/L_{bed} = 0.15, \text{0D} \]

gas temperature

\[ \frac{\text{gas vapor content}}{T_g} \]

Effect of bed aspect ratio

\[ \frac{L_0}{L_{bed}} = 0.65, \text{TFM} \]
\[ \frac{H_0}{L_{bed}} = 0.65, \text{0D} \]
\[ H_0/L_{bed} = 0.15, \text{TFM} \]
\[ H_0/L_{bed} = 0.15, \text{0D} \]

\[ \text{gas vapor content} \]

\[ T_g \]

\[ \text{time [s]} \]

\[ \text{LoD/LoD_{max}} \]

\[ \text{time [s]} \]
Conclusions and outlooks

Development of a **0D model** based on the results of **TFM simulation**

Formation of two **phenomenon-specific zones**

Quantification of “**well-mixed-ness**” via the **degree of uniformity** for LoD and temperature

demonstration of the 0D model validity on fulfilling the criteria for “**well-mixed**” condition

**Validation** and integration of **cohesion** comes next
Thank you for your attention!
Open PhD Positions for „MATHGram“

- **Topic:** particles + heat
- **Lead:** Prof. Charley Wu (Univ. Surrey)
- **15 PhDs across Europe**
- **Starts 2019**
- **2 PhDs in wonderful Austria (Graz/Linz/Vienna)**
- **Apply now!** (ippt.turaz.at/jobs, cfdem.com)

https://www.graztourismus.at
Benchmarking a Novel 0-D Model Against Data from Two-Fluid Model Simulations of a Wet Fluidized Bed

Stefan Radl, Mohammadsadegh Salehi
Institute of Process and Particle Engineering, Graz University of Technology

Maryam Askarishahi
Research Center Pharmaceutical Engineering GmbH, Graz

radl@tugraz.at