The MP-PIC method for CFD-simulation of fluidized beds – Comparison of two different implementations

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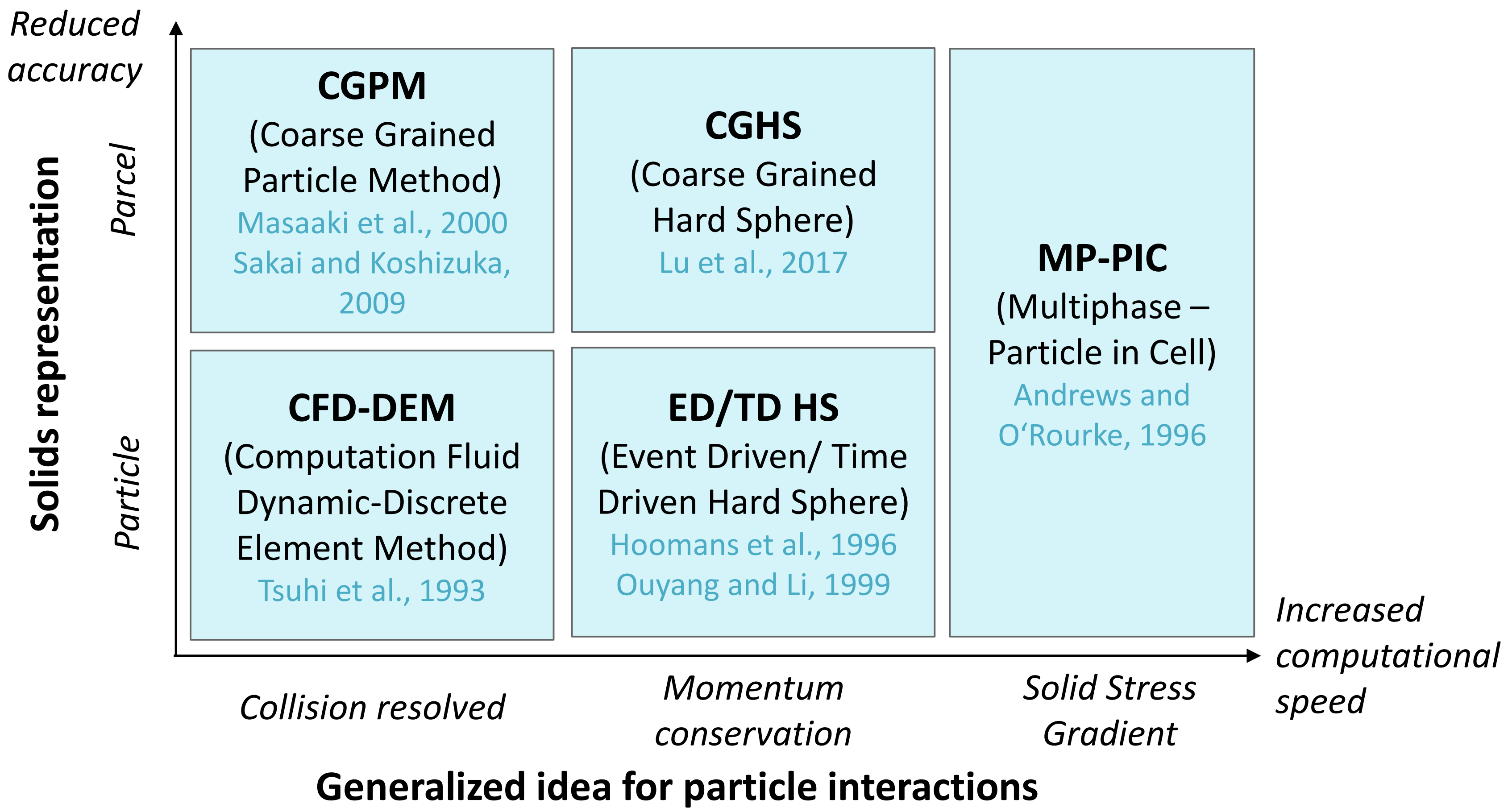
Computational speed vs. accuracy

– Large-scale systems (e.g. combustors) involving up to 10^{18} particles are time-intensive to model
  - ➢ Tradeoff between computational speed and accuracy for the simulation of fluidized beds



[1] Lu et al. (2017): *Ind. Eng. Chem. Res., 56 (27)*

Methodology

Software implementation

Barracuda VR® 17.3

- Proprietary software by CPFD Software LLC
- Solver for compressible fluids
- Structured grid

OpenFOAM® v6

- Open source software by The OpenFOAM Foundation Ltd
- Solver for incompressible fluids
- Unstructured grid

Different software – Identical results?

Particle stress

- Explicit inter-particle stress model according to Harris and Crighton [2]

$$\tau = \frac{P_s \cdot {\alpha_p}^{\beta}}{\max\left[\alpha_{cp} - \alpha_p, \beta \cdot (1 - \alpha_p)\right]}$$

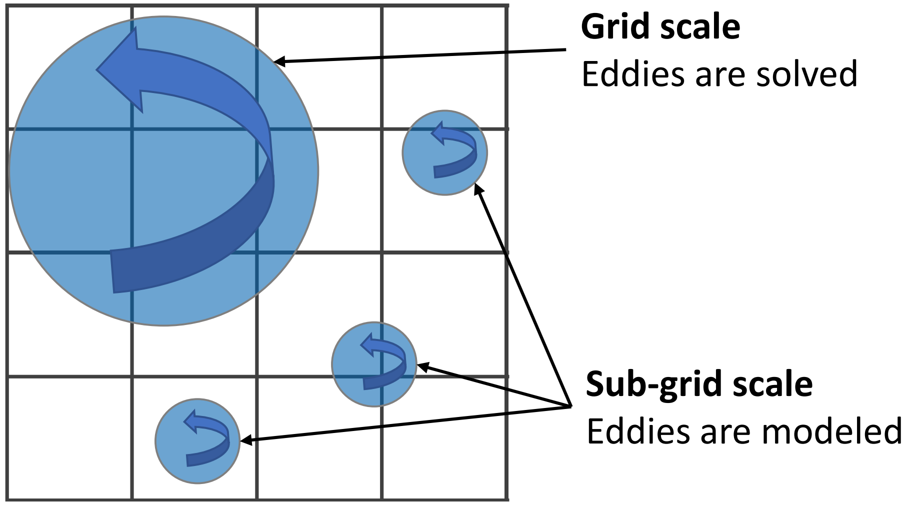
τ	Inter-particle stress
P_s	Modeling constant
α_p	Particle volume fraction
α_{cp}	Particle volume fraction at close-pack
β	Modeling constant

Turbulence model

- Large Eddie Simulation (LES) according to Smagorinsky [3]
  - ➢ Resolving large length scales, but model smallest length scales to reduce the computational costs

Drag model according to Gidaspow [5]

- Combination of approaches by Wen and Yu [6] and Ergun [7]
- Homogeneous drag model commonly used in literature



Schematic representation of the LES [4].

[2] Harris and Crighton (1994): *Journal of Fluid Mechanics, 266*.
[3] Smagorinsky (1963): *Monthly Weather Review, 91*.
[4] Sagaut (2006): Large Eddy Simulation for Incompressible Flows, *Springer*.
[5] Gidaspow (1994): Multiphase Flow and Fluidization, *Academic Press*.
[6] Wen and Yu (1966): *Chemical Engineering Progress Symposium Series, 62*.
[7] Ergun (1952): *Chemical Engineering Progress, 48*.

Simulation Setup

Lab-scale reactor

Geometry

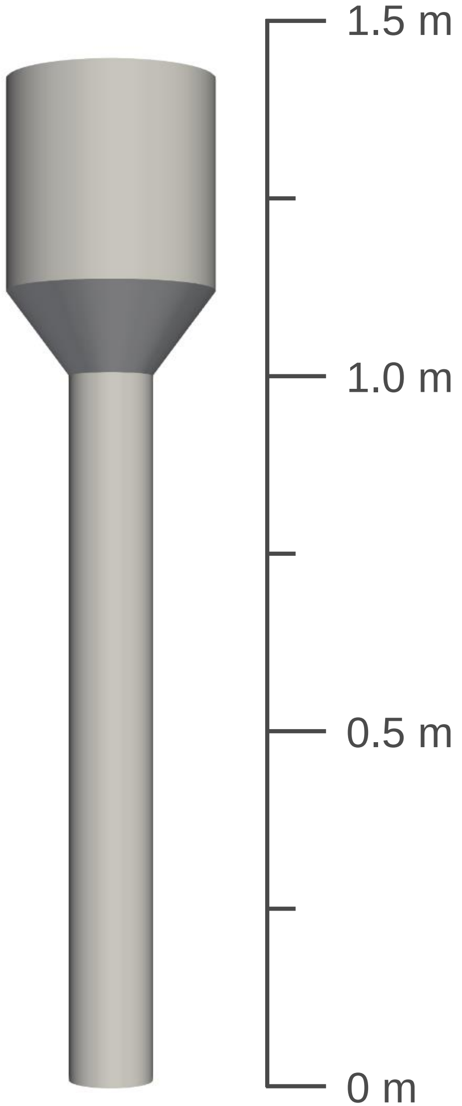
– Height: 1.4 m, diameter: 0.1 m

Material: Quartz sand (Geldart B)

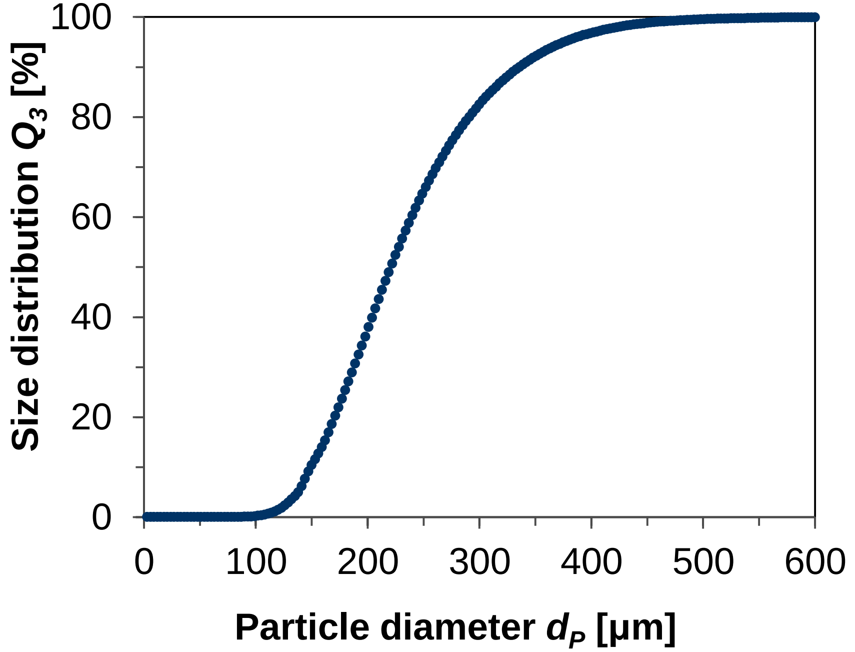
– Initial bed height: h_{bed} = 0.1 m
  - ➢ Bed mass: m_{bed} = 1.1 kg
– Solid density: ρ_s = 2600 kg/m^3
– Close pack fraction: α_{cp} = 0.54
– Sauter diameter: d_{32} = 220 µm

Process conditions

– Isothermal flow (300 K)
– Velocity range from bubbling to turbulent fluidization
  - ➢ u_g = 0.21 – 1.33 m/s



Geometry of the lab-scale reactor.



Measured particle size distribution of F34 quartz sand.

Results

Lab-scale reactor

Key Parameter: Solids concentration averaged over the cross-section and over time using the pressure drop

$$\varepsilon_s = \frac{dp/dz}{\rho_s \cdot g}$$

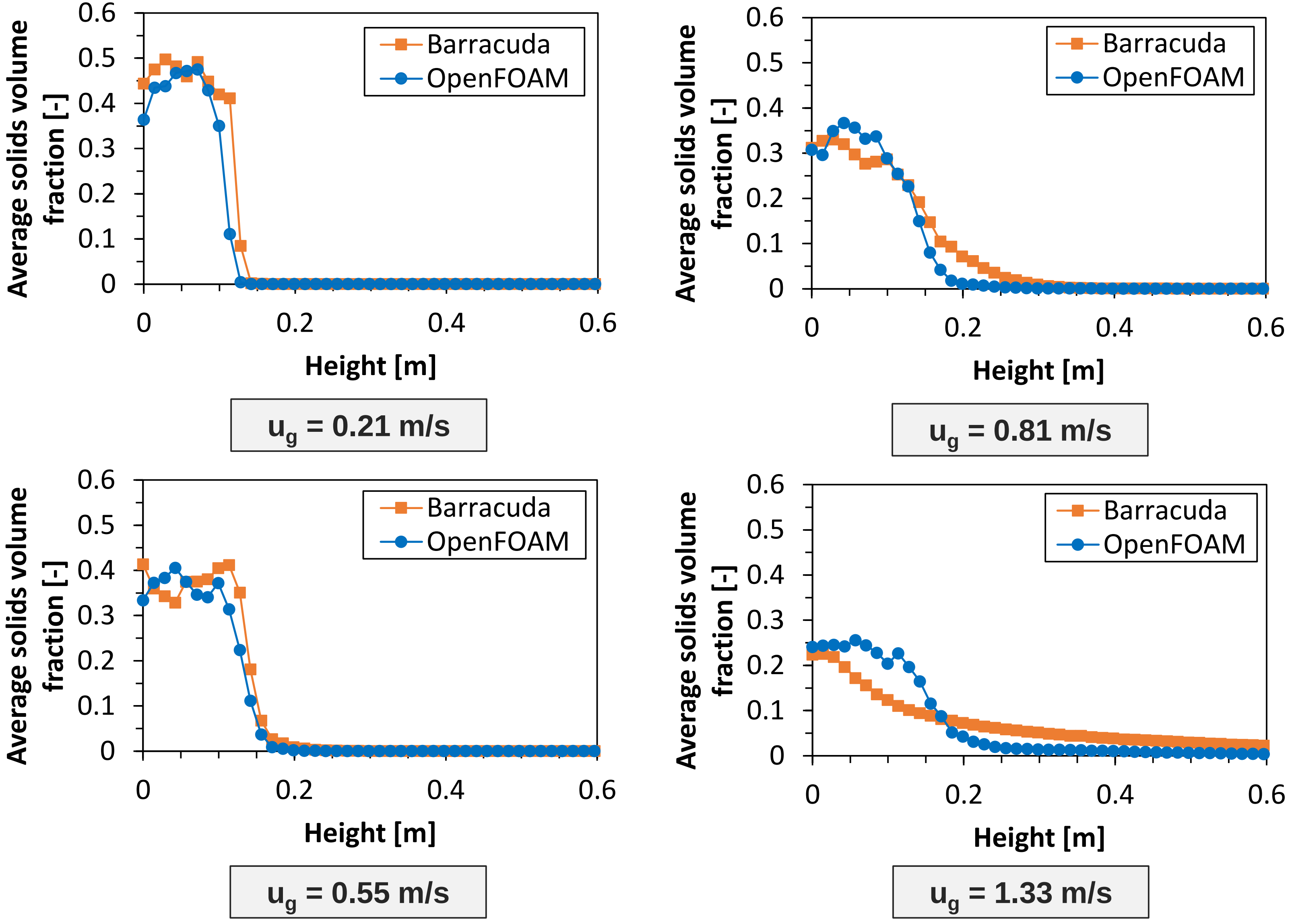
– Similar results for low velocities

– Diverging results with increasing velocities

➢ Error of pressure drop increases with increasing velocity

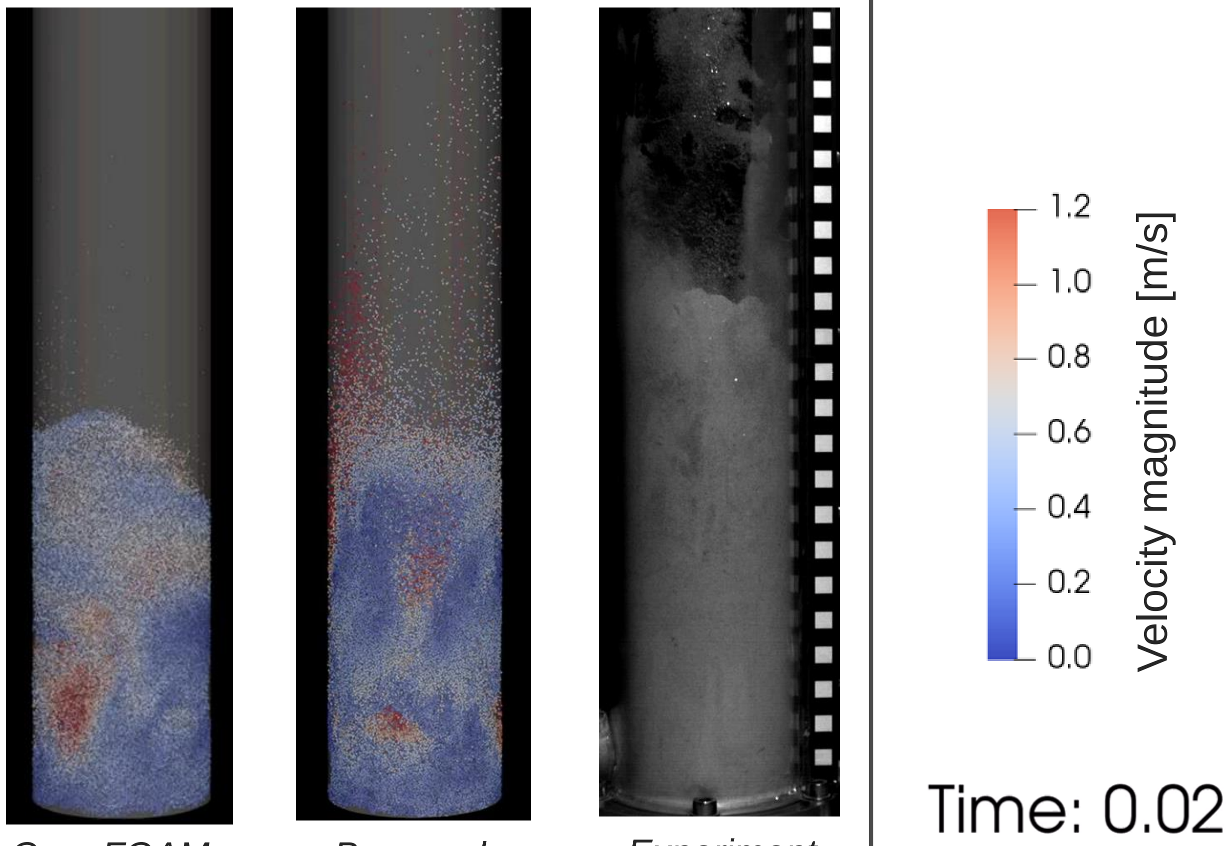
Table 1: Relative error of calculated mass (OpenFOAM).

Velocity [m/s]	**Calculated mass** [kg]	**Relative error**
0.21	1.045	4.98 %
0.55	1.031	6.29 %
0.81	1.009	8.24 %
1.33	0.925	15.94 %



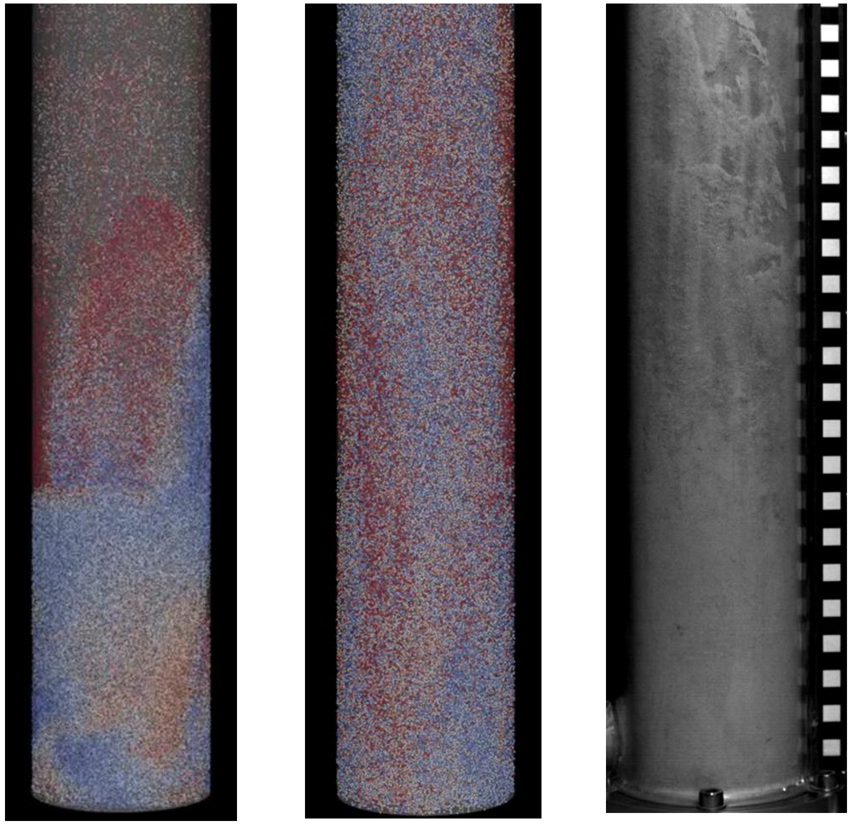
Comparison of video recordings: Recording frequency 50 Hz slowed down to 10 fps

u_g = 0.55 m/s



OpenFOAM *Barracuda* *Experiment*

u_g = 1.33 m/s



OpenFOAM *Barracuda* *Experiment*

Geometry [8,9,10]

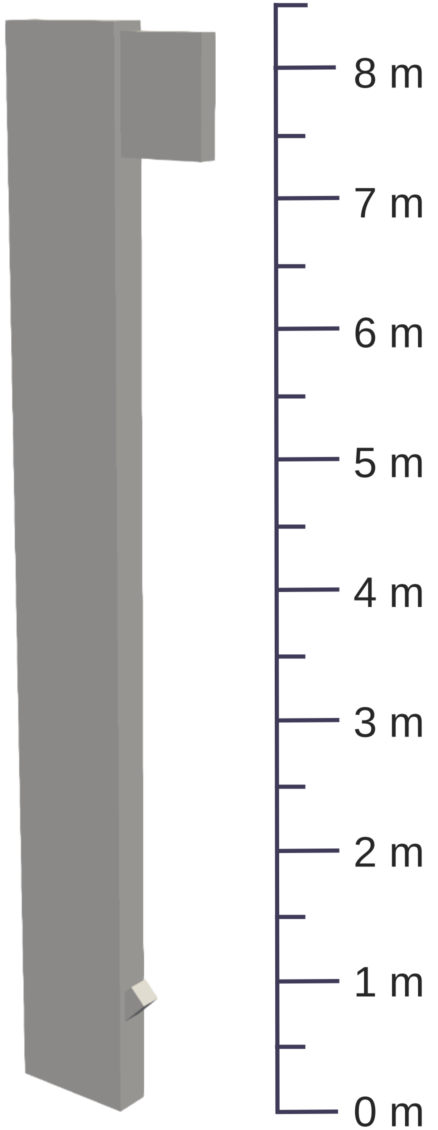
- Height: 8.35 m, cross-section: 1 m x 0.3 m

Material: Quartz sand (Geldart B particles) [8]

- Initial bed mass: $m_{bed} = 300$ kg
- Solid density: $\rho_s = 2600$ kg/m^3
- Sauter diameter: $d_{32} = 150$ µm

Process conditions

- Fluid velocity: $u_g = 3$ m/s (isothermal flow at 300 K)
- External circulation rate G_s is adjusted to result in a constant solid hold-up around 300 kg
  - ➢ Experimental circulation rate: $G_s = 20$ kg/(m^2·s) [8]



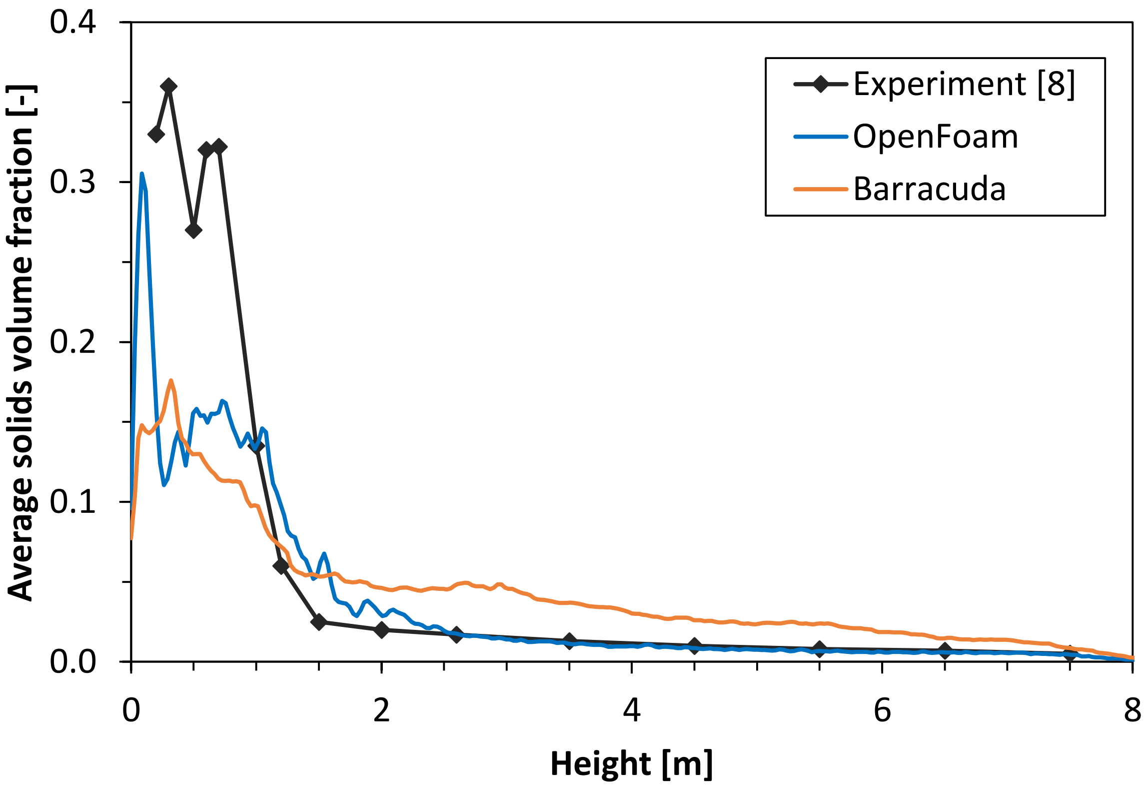
Geometry of the pilot-scale reactor.

[8] Schlichthärle (2000): *Doctoral thesis*, TUHH.
[9] Hartge et al. (2009): *Particuology, 7*.
[10] Chen et al. (2013): *Powder Technology, 235.*

Results
Pilot-scale reactor

- Simulated solids fractions too low in bottom zone
- Barracuda predicts a more homogeneous axial distribution than OpenFOAM
- External circulation rates are adjusted to obtain a constant solid hold-up of 300 kg
  - ➢ $G_{s,exp}$ = 20 kg/(m²·s) [8]
  - ➢ $G_{s,OF}$ = 17 kg/(m²·s)
  - ➢ $G_{s,BC}$ = 46 kg/(m²·s)

Data	Solid hold-up [kg]	Pressure drop [mbar]
Experimental [8]	300	99
Barracuda	300	87
OpenFOAM	300	73



- ➢ **Lower pressure drop with OpenFOAM but more homogeneous axial distribution with Barracuda**
- ➢ **Better agreement of external circulation rate with OpenFOAM**

[8] Schlichthärle (2000): *Doctoral thesis*, TUHH.

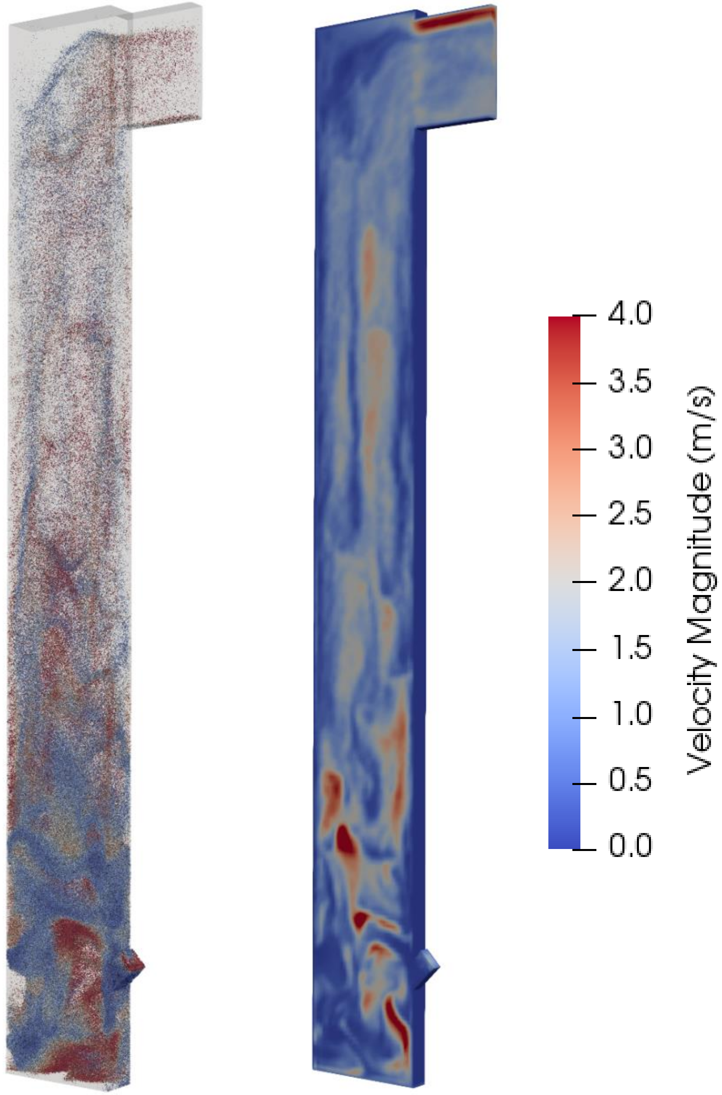
Summary

The MP-PIC method for CFD-simulation of fluidized beds

- Both implementations can predict fluidization behavior at lower fluidization velocities with reasonable agreement
- Both implementations under-predict the resulting pressure drop
  - ➢ Relative error increases with increasing velocity
- Despite the same conditions significant differences between OpenFOAM and Barracuda
  - ➢ Lower fluidization intensity and pressure drop with OpenFOAM compared to Barracuda
  - ➢ More realistic segregation of particles and external circulation rate with OpenFOAM

Next step:

➢ Implementation of EMMS based drag model for a better agreement with the experimental data



Instantaneous velocity magnitude of the particles (left) and the fluid (right) in the pilot-scale riser (OpenFOAM).

Thank you for your attention!

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DFG Deutsche Forschungsgemeinschaft

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