Three-dimensional full-loop simulation of cold gas-solid flow in a pilot-scale dual fluidized bed system - a preliminary study

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Outline

- OxyCrack project
- Pilot-scale facilities
- CPFD simulations
  - Preliminary results
  - Challenges and experiences with Barracuda VR
- Conclusions

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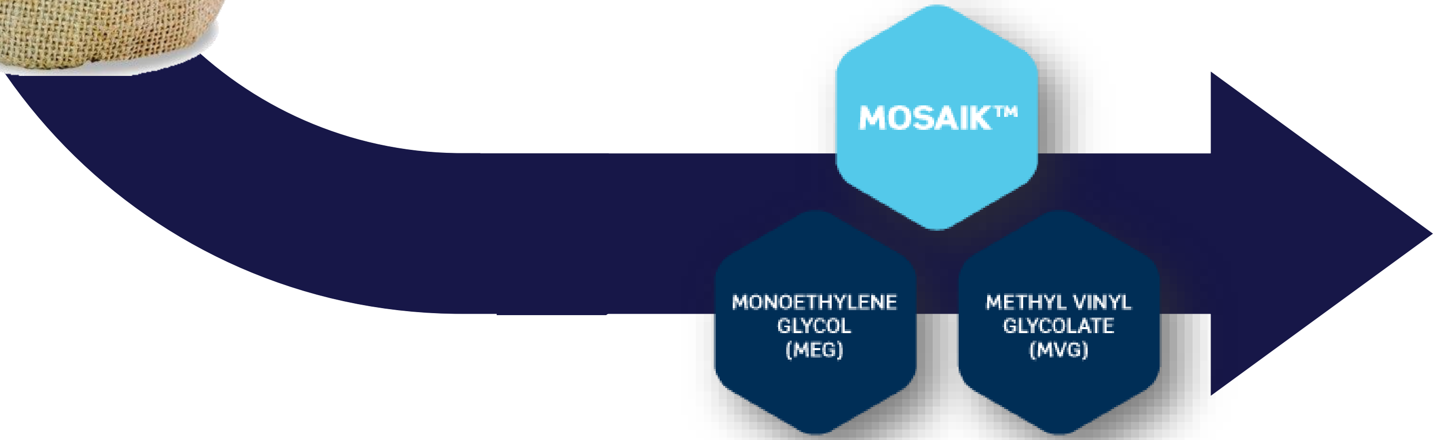
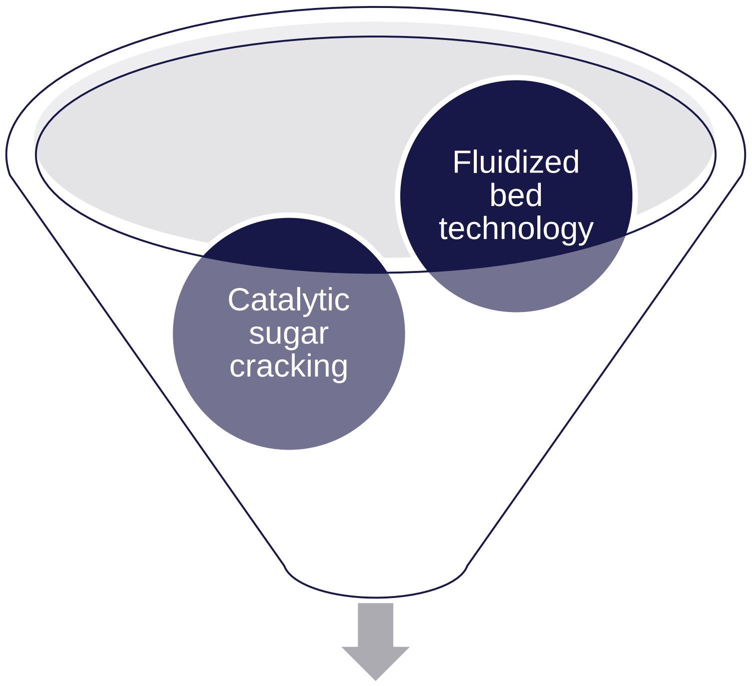
Catalytic cracking of sugars

- Novel technology for producing glycolaldehyde-rich oxygenates to be further converted to bio-based materials.
- The MOSAIK^{TM} HT cracker will enable conversion of sugars (e.g. sucrose, dextrose, and second-generation) into intermediate products such as monoethylene glycol (MEG) or methyl vinyl glycolate (MVG).
- MEG is used in PET plastic bottles, polyester fibres, food packaging etc. and can be produced in a cost-efficient way using the MOSAIK^{TM} HT cracker.



Catalytic cracking of sugars



Cost-efficient alternative to fossil-based MEG

- Challenging to make the catalytic conversion in an efficient way.
- Combining catalytic cracking and fluidized bed technology provides an alternative to current production methods from fossil-based feedstocks; naptha, gas, or coal.
- Circulating fluidized beds!

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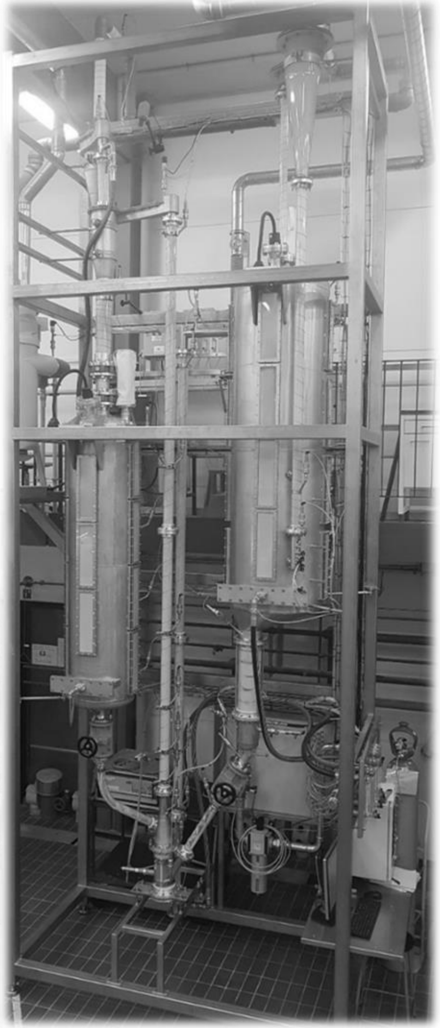
Motivation for pilot-scale facilities

- Cold- and hot-flow pilot-scale CFB's of a dual fluidized bed configuration have been build at DTU and HT.

<u>Why?</u>

- Intermediate step for scale-up of the technology.
- Provides and opportunity to understand hydrodynamics and chemistry.
- Risk mitigation in terms of troubleshooting and problem solving of potential full-scale issues at a cheaper pilot-scale level.
- Input for validation of CFD model under controlled and flexible operating conditions.

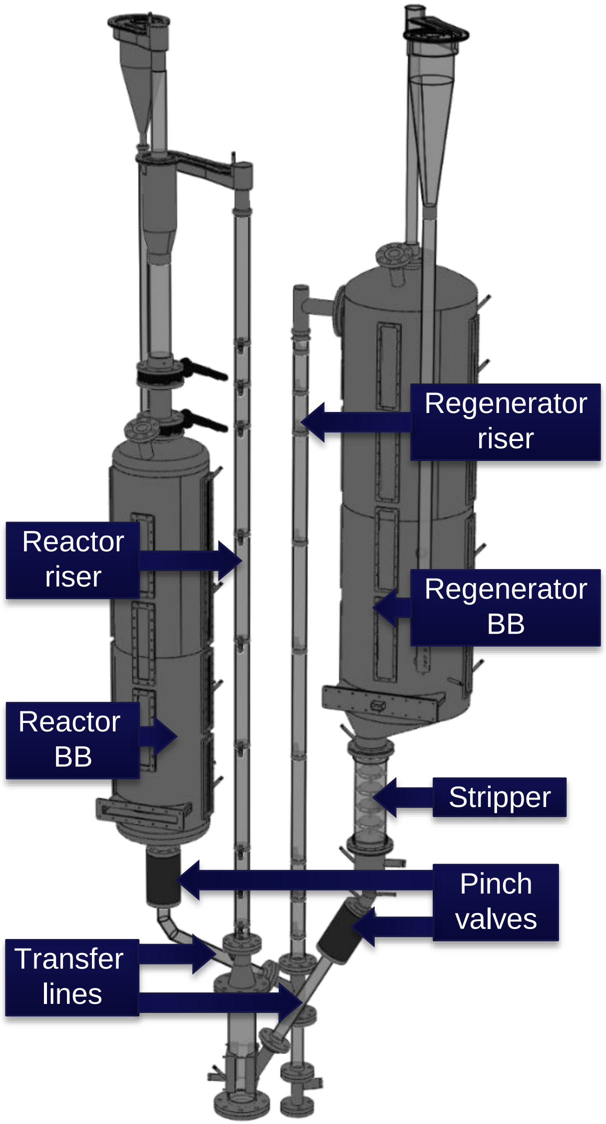
Haldor Topsøe hot-flow pilot-scale system



DTU cold-flow pilot-scale system

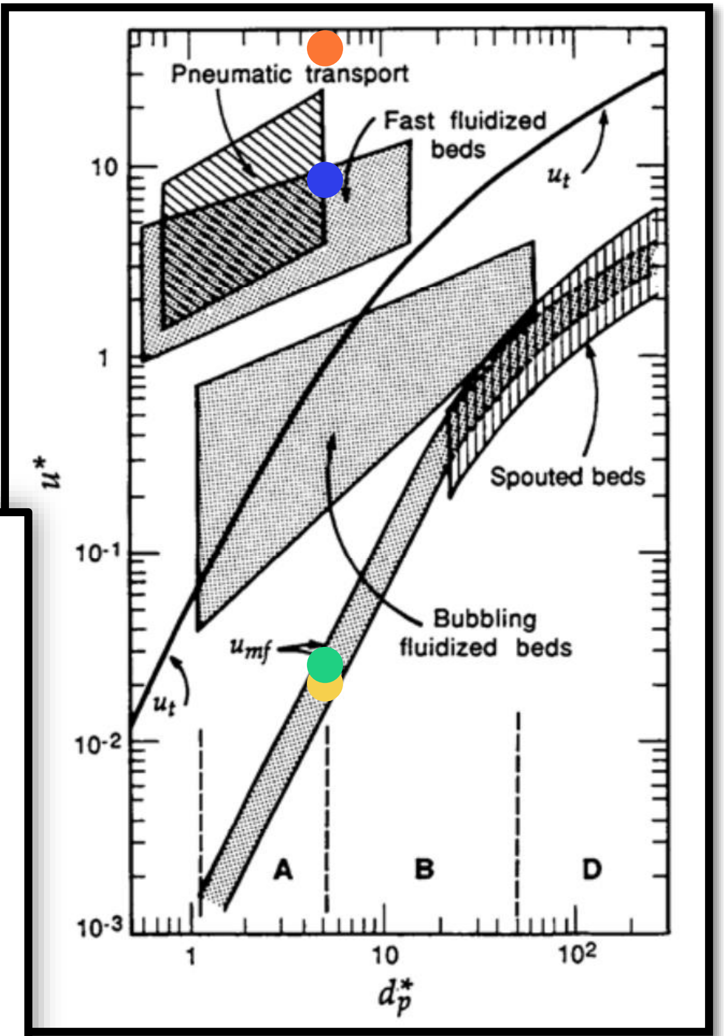
Cold-flow setup

- System consists of a reactor loop and regenerator loop.
  - Risers
  - Bubbling beds (BB)
  - Cyclones
  - Stripper
  - Transfer lines
  - Pinch valves
- Solids flow rate is controlled by pinch valves in the transfer lines.
- Bubbling beds are equipped with spargers to fluidized the bed inventory.

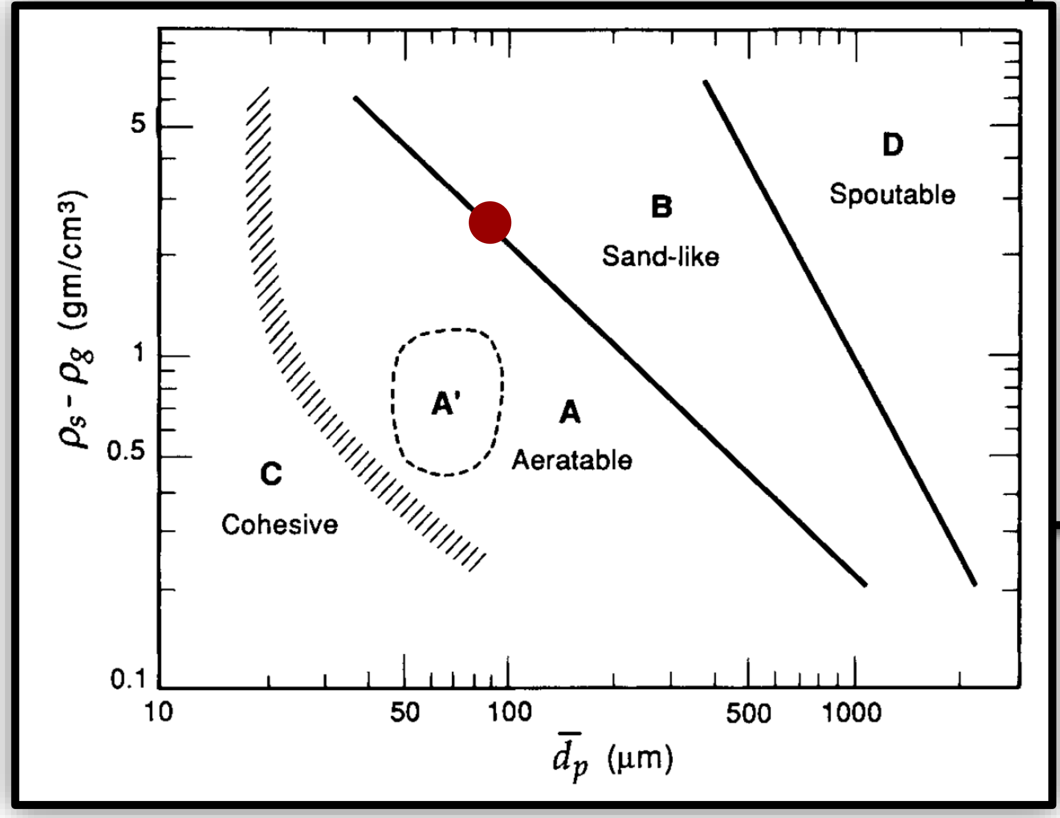


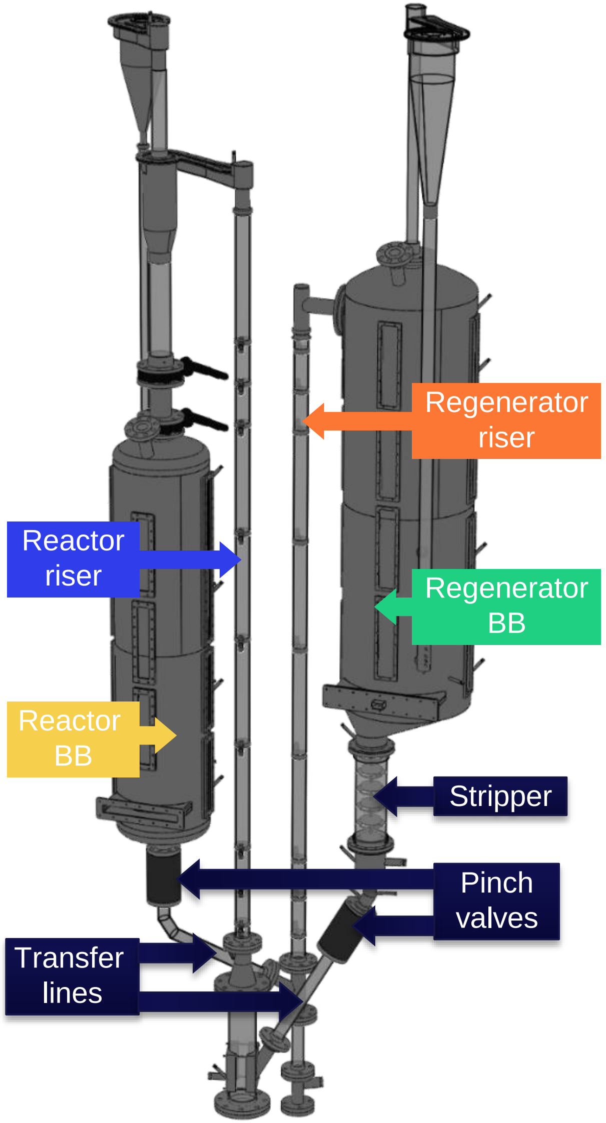
Cold-flow setup

Kunii, D., & Levenspiel, O. (1969). *Fluidization engineering* (2nd ed.). Wiley.



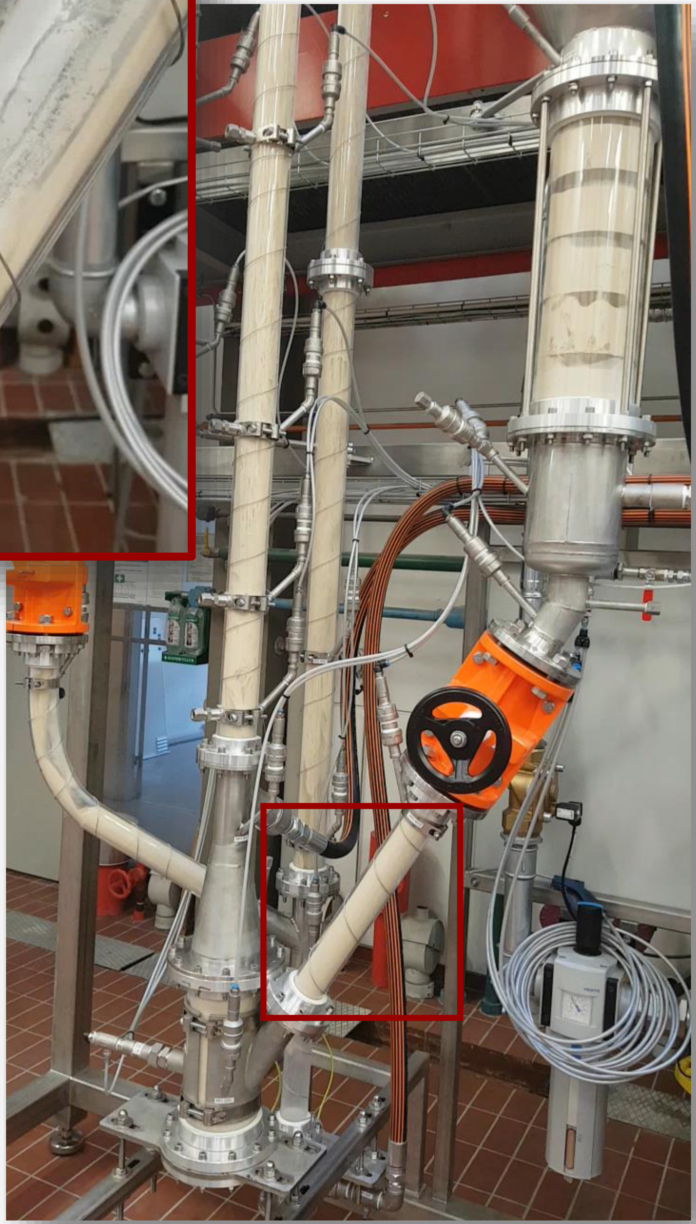
$$d_p{}^* = Ar^{1/3}, u^* = \frac{Re_p}{Ar^{1/3}}$$

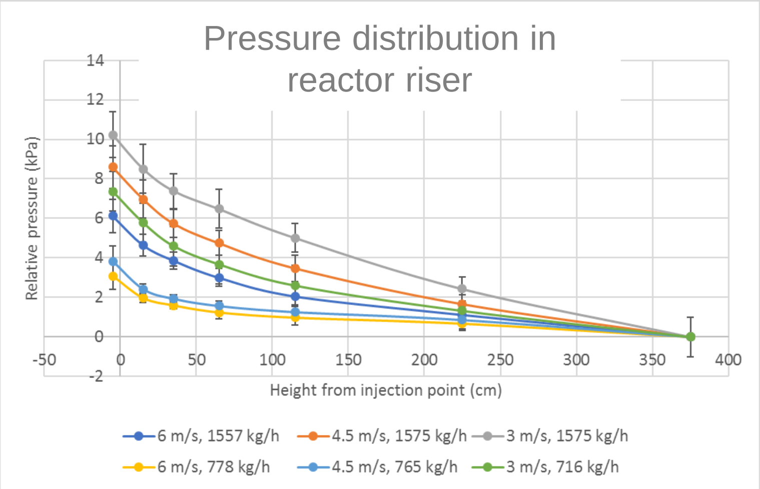


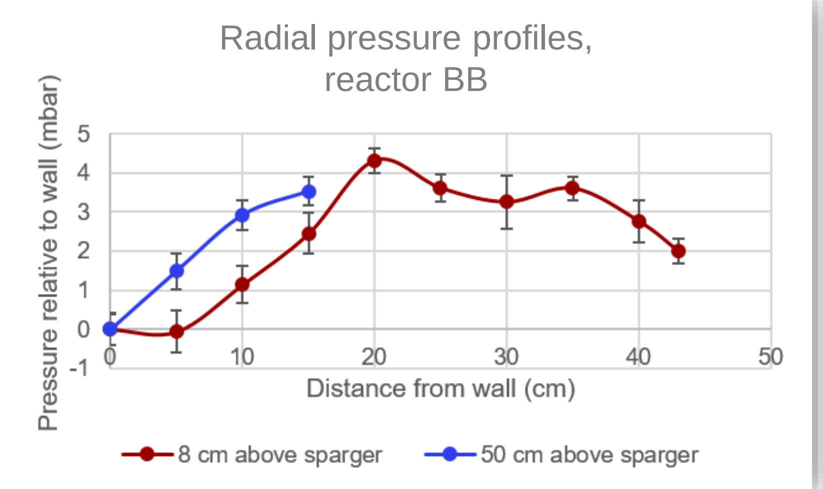


Cold-flow setup

- Video of solids flow in the system during operating at high solids flow rate (2200 kg/h).
- We are able to conduct:
  - pressure measurements throughout the system,
  - measurements of solids circulation rate,
  - quantification of stripper efficiency,
  - radial pressure measurements in the bubbling beds,
  - and RTD measurements in the risers.







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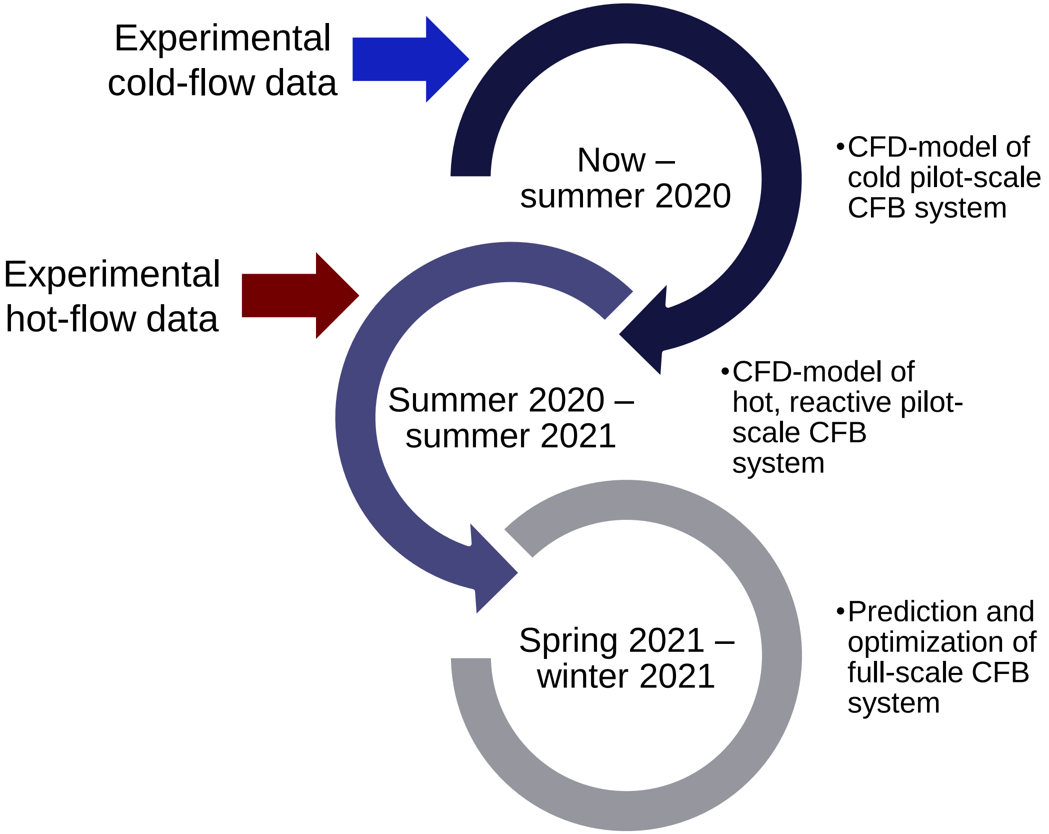
CPFD simulations

Ph.D. study to:

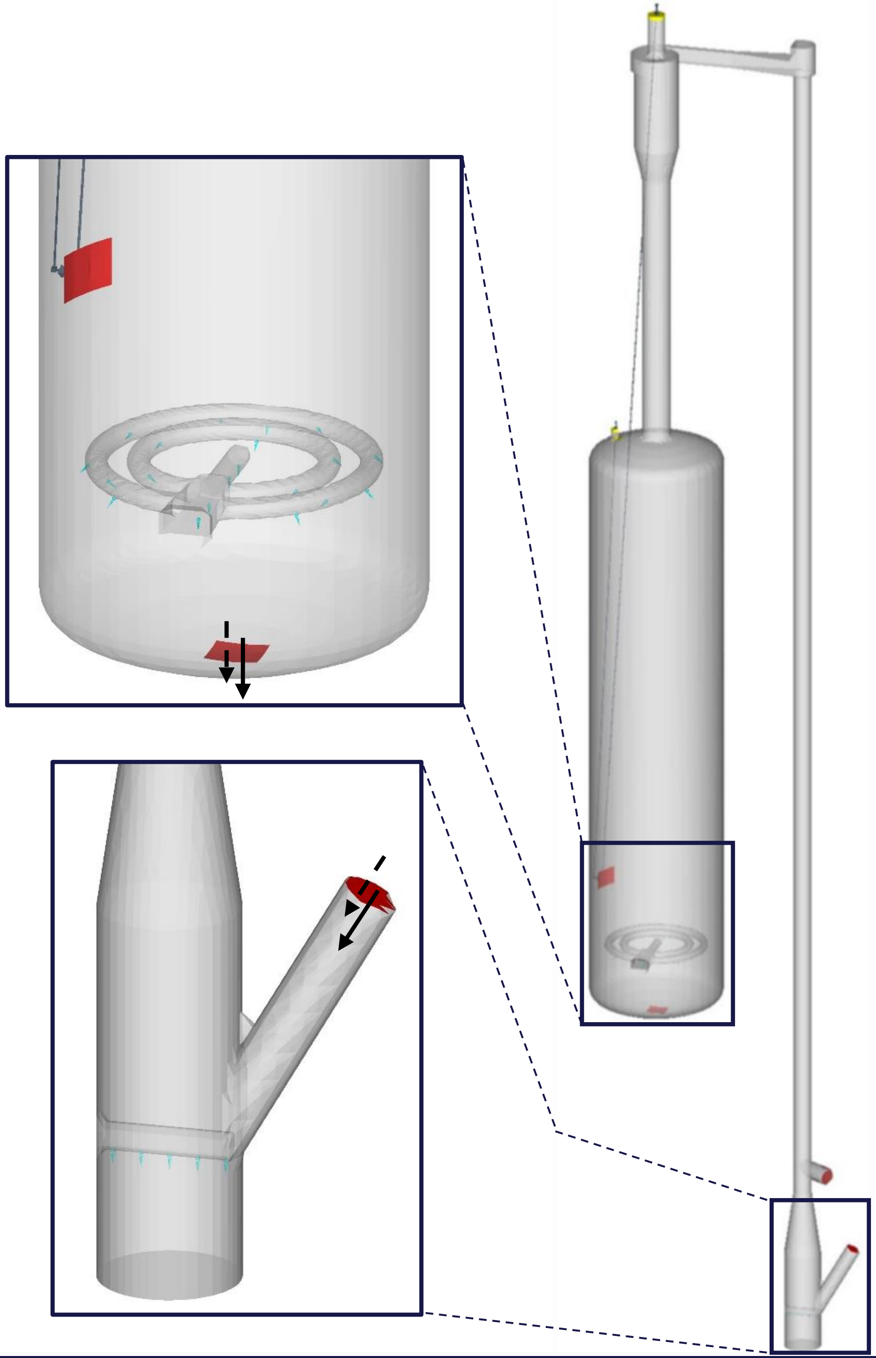
- improve understanding of the hydrodynamics of a CFB system for catalytic cracking of sugars,
- develop a computational fluid dynamics (CFD) model, describing the hydrodynamics and chemical reactions in the system,
- add a parallel path to the developement process,
- and bridge the gap between pilot- and commercial-scale (risk mitigation).



CPFD simulations - setup

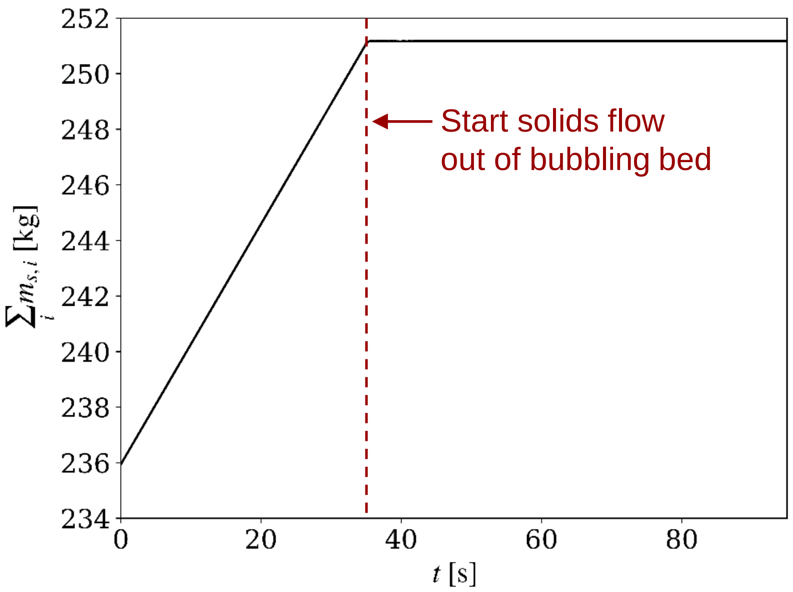
- Reactor ”loop” is modeled using Barracuda VR17.4.0.
- Excerpt of transfer line is included while pinch valves are disregarded.
- BC connectors to recycle solids exiting the cyclone and bypass line (secondary cyclone is neglected).
- ”Out-of-the-box” simulation.

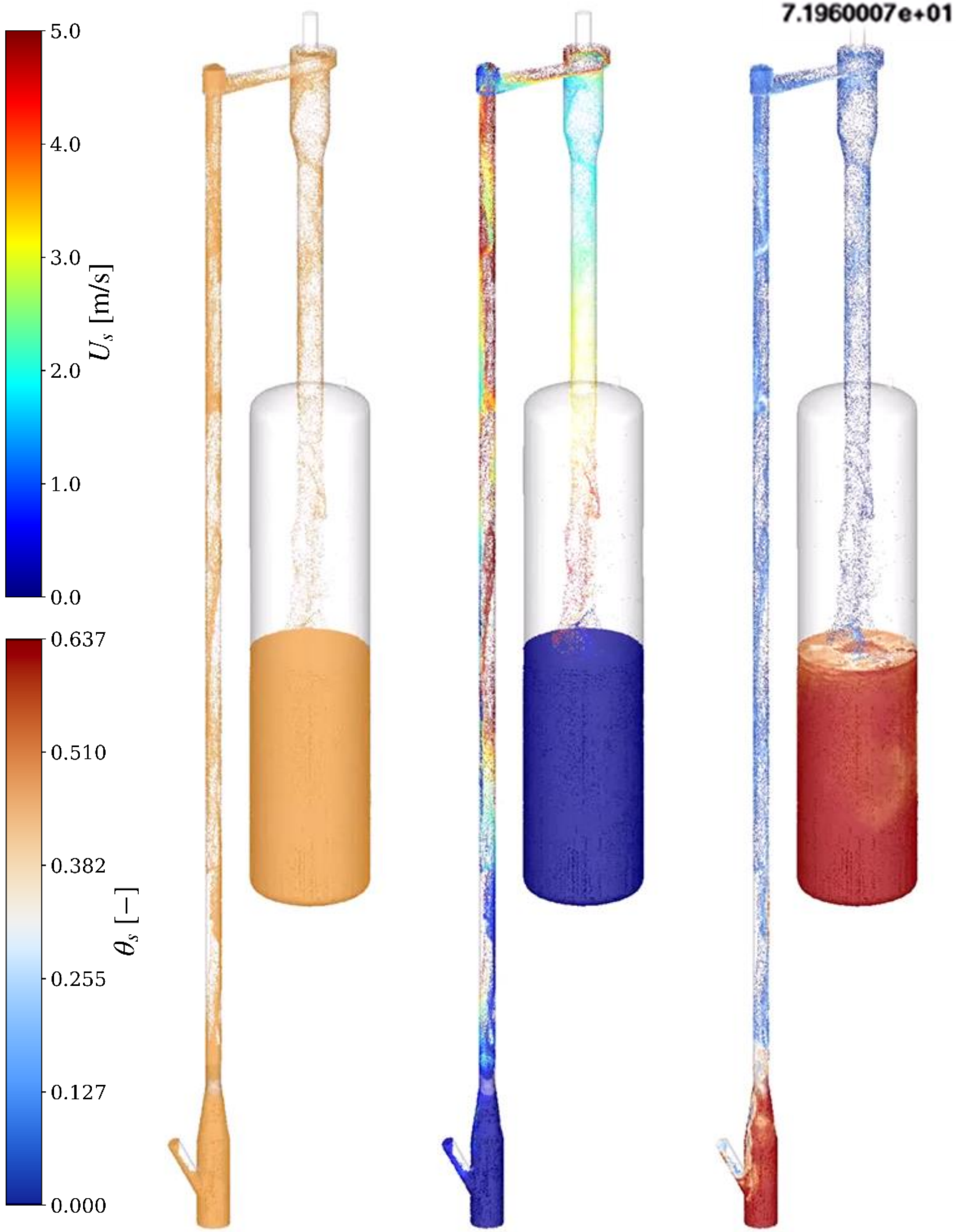
Number of numerical particles (parcels)	4.5e+06
Number of particles per parcel	6.8e+04
Number of grid cells	2.6e+05
Average grid size	$125D_p$
Simulation time	95 s
Averaging time	50 s



CPFD simulations - results

- Catalyst movement in system is animated on the right.
- Oscillations in solids flow rate through the riser.
- Mass of system is maintained at the desired value using the inflow BC at the bottom of the bubbling bed with a specified outflow of solids per unit time.

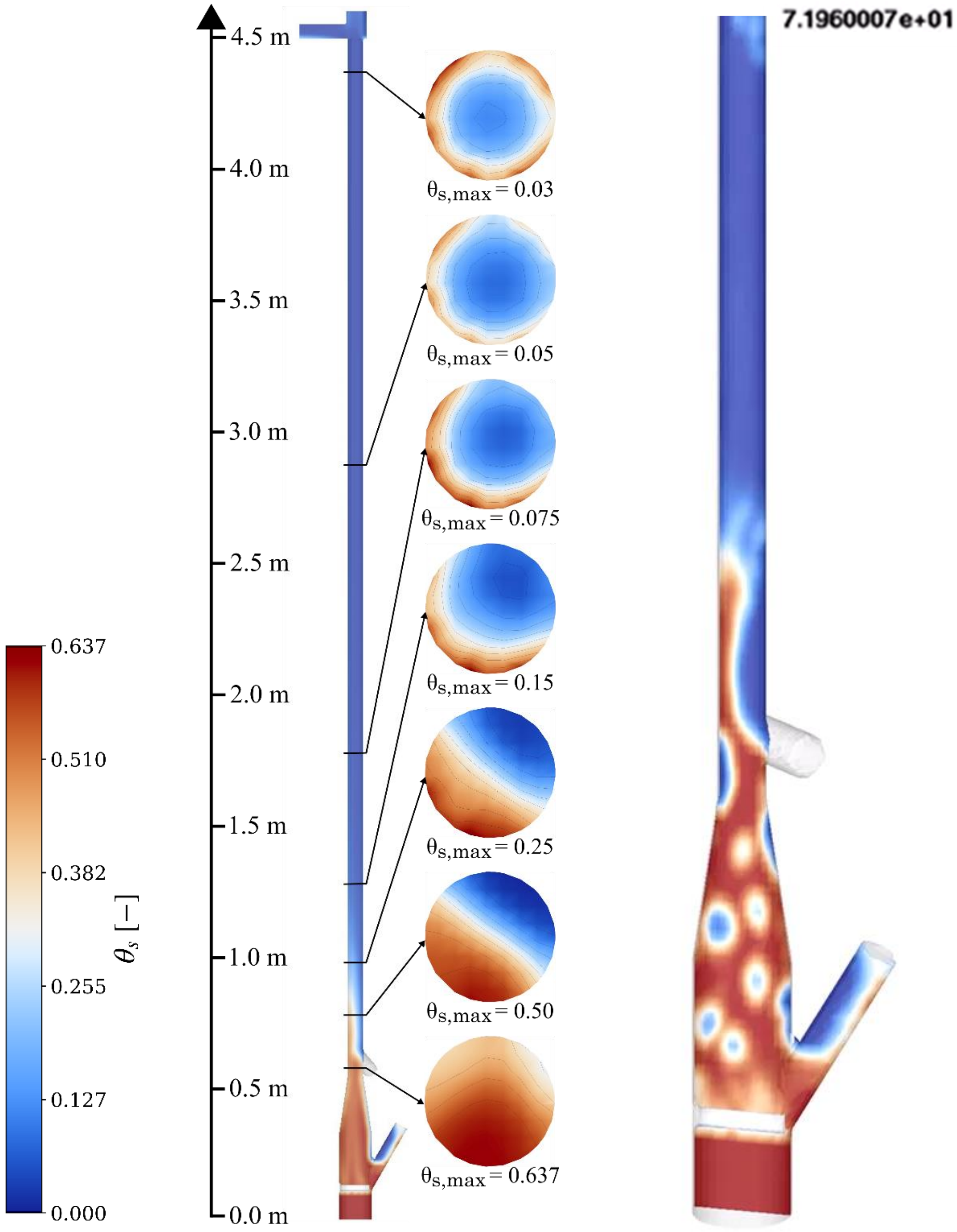


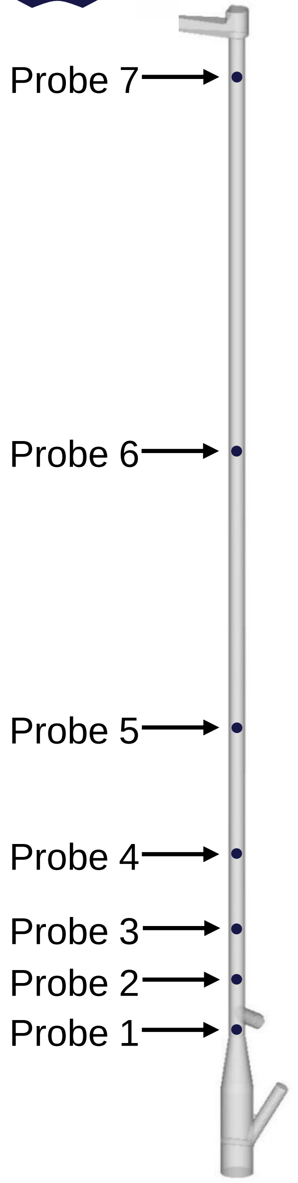


CPFD simulations - results

Reactor riser

- Increased aeration in transferline to ensure stable inlet solids mass flow rate.
- Build-up of particles in the conditioning zone and subsequent upward conveying.
  - Skewed radial solids concentration profile in the lower part of the riser.
  - Core-annulus radial solids concentration profile in upper part of riser.
- No downward flow of solids near riser wall predicted by the model.

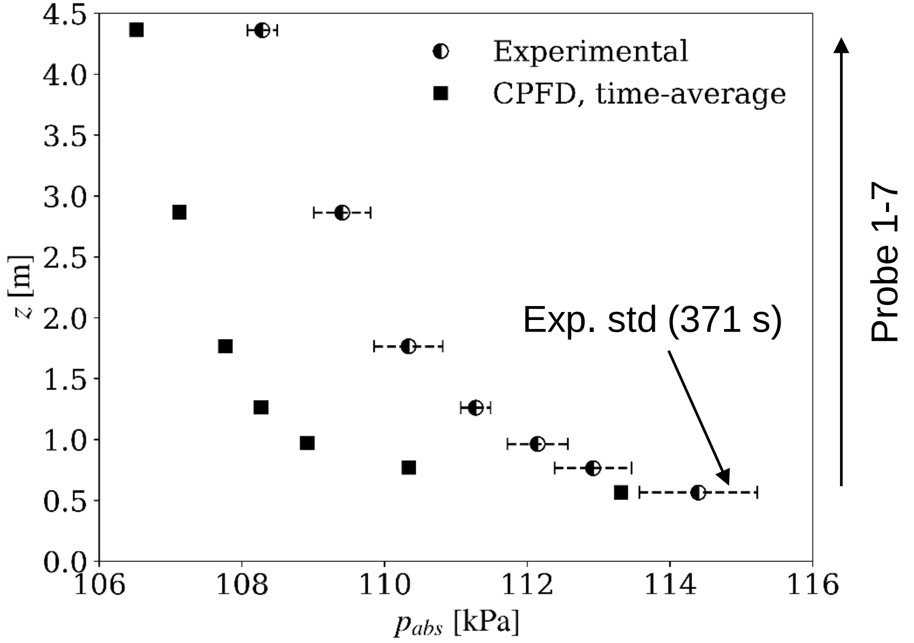


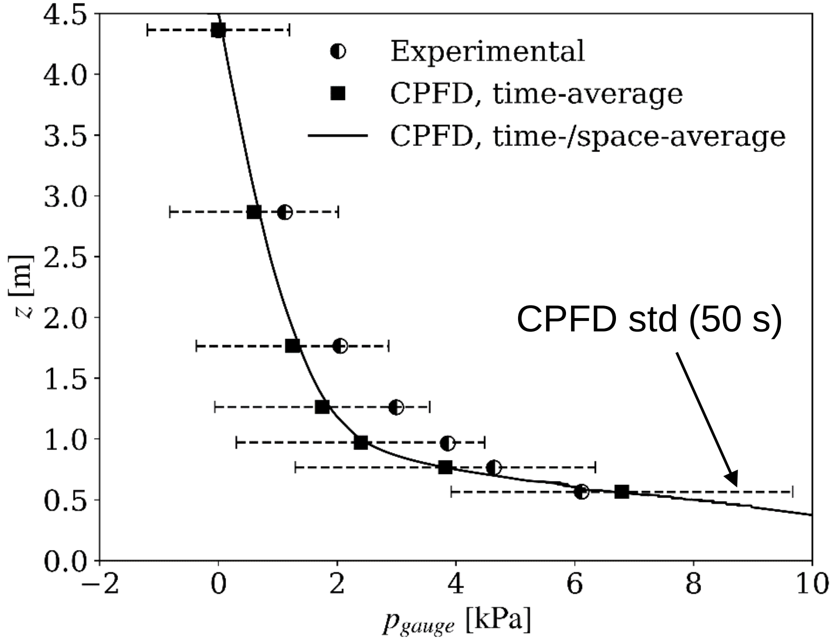


CPFD simulations - results

Reactor riser

- Overprediction of pressure drop in the conditioning zone and bottom part of the riser.
- Large temporal fluctuations in numerical wall probe pressure signals.
- Sensitivity to outlet pressure at cyclone.

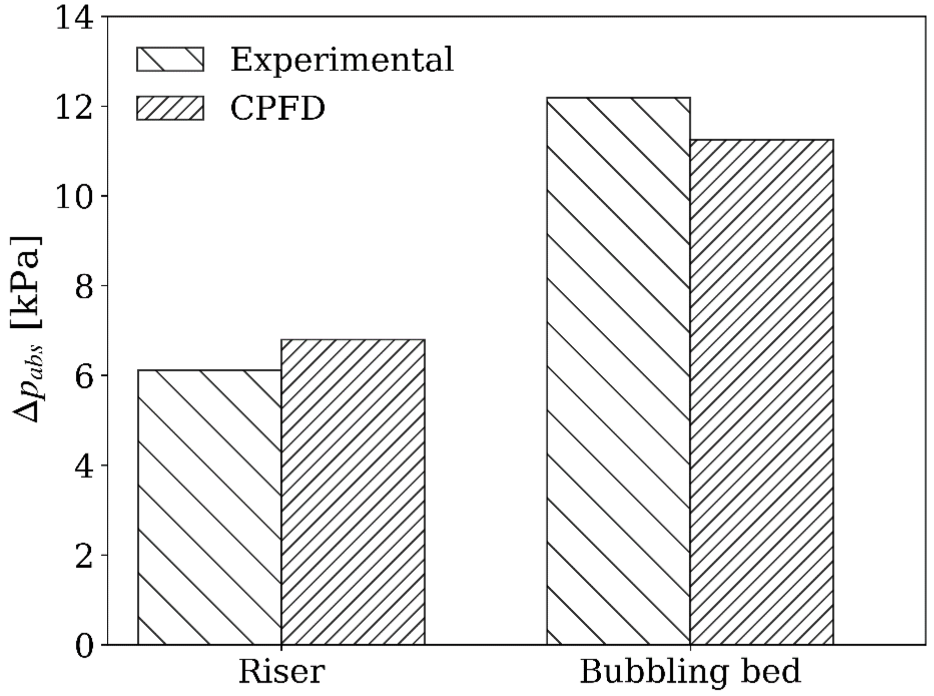




CPFD simulations - results

Reactor riser

- Overprediction of pressure drop in the conditioning zone and bottom part of the riser.
- Large temporal fluctuations in numerical wall probe pressure signals.
- Sensitivity to outlet pressure at cyclone.
- Acceptable prediction of the overall pressure drop across the height of the riser.
  - And bubbling bed.



CPFD simulations – challenges and experiences

- Boundary conditions.
  - How to obtain these from experiments?
  - How to ensure proper implementation in CPFD?
- Pinch valve modeling.
- Drag model selection.
- Validation.

- Capturing complex (or even simple, but small internal geometries).
- Resolving flow of fluid point source injections.
- Limited options for selection of turbulence models for dilute flows.
- Lack of model for turbulent dispersion of particles.

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Conclusions

- Barracuda VR is to be used in simulating a full-loop pilot-scale dual fluidized bed in both cold and hot (reactive) conditions.
- A preliminary study has been conducted to indentify challenges of modeling such system in Barracuda VR.
- Results of the preliminary study of the reactor ”loop” suggest that the ”out-of-the-box” simulation approach yields acceptable results with respect to trend and overall behavior predictions.
- Pinch valves are a major modeling challenge in achieving the desired model.
- Additional modeling will have to be conducted to solve the pinch valve challenge and improve model accuracy through:
  - appropriate drag model selection,
  - sensitivity studies of mesh size, number of particles, time-step, solver coefficients etc.,
  - and improved boundary conditions.

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Questions?

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