Validation and Comparison of CFD-DEM and MP-PIC Simulations of a Gas-Fluidised Bed using Positron Emission Particle Tracking

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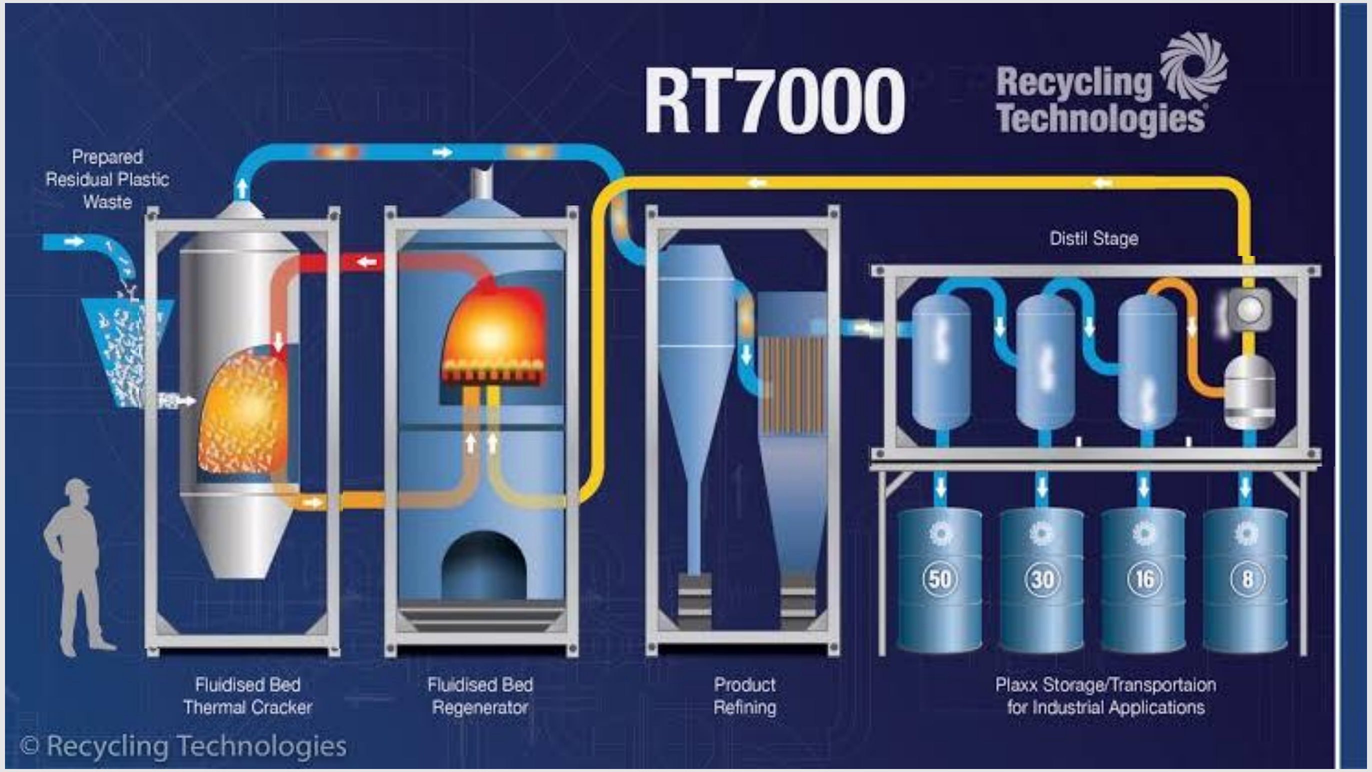
Plastic Waste - A Global Challenge

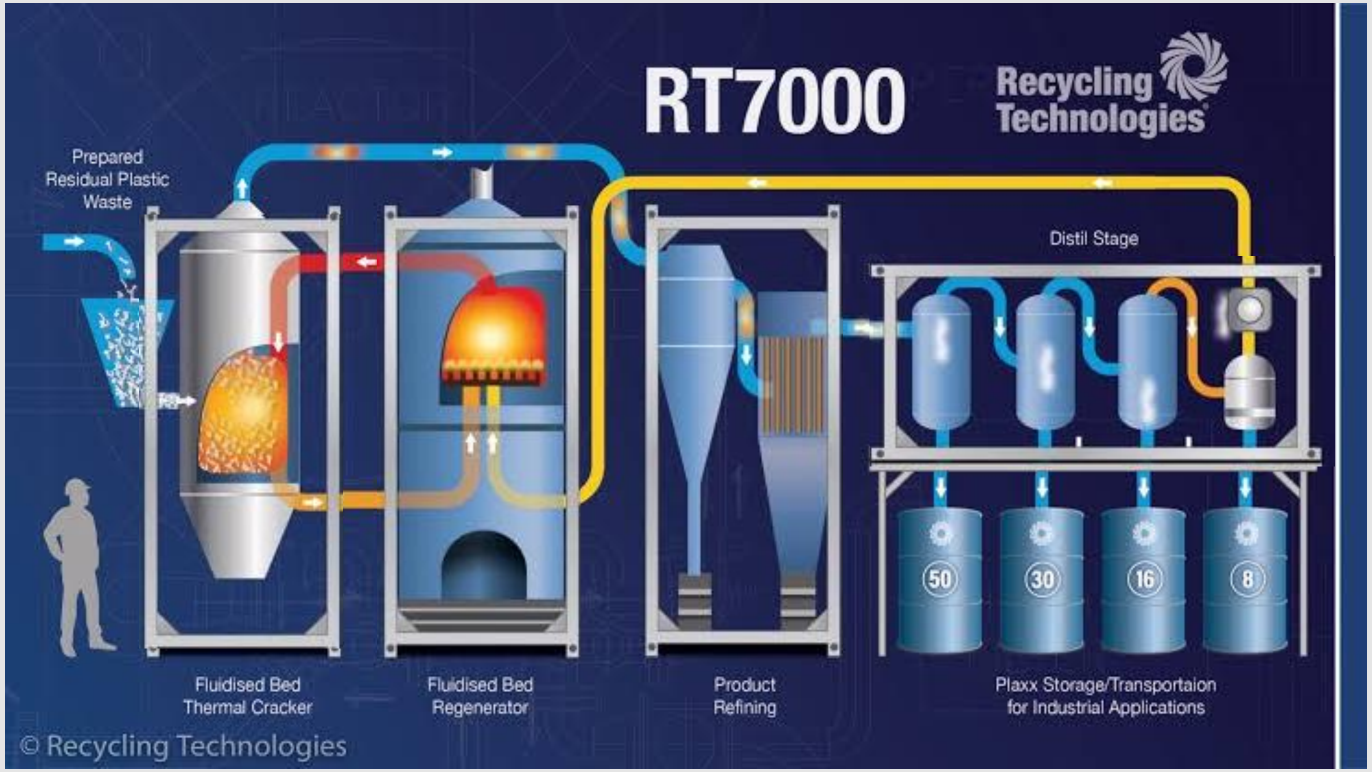
- **~400 million tonnes** per annum produced.
  - Equivalent to the mass the human population every 1.5 years
- 91% of plastic is **not recycled**
- Of the 9% that *is* nominally recycled, the majority forms **low-quality** second-life products.

Waste Plastic Pyrolysis



- Working with industrial partner Recycling Technologies Ltd.
- Efficiently convert plastic waste into **valuable petrochemical feedstocks and fuels**.
- Fluidised bed technology allows **large-scale processing**.

Waste Plastic Pyrolysis



Modular design minimises transport.

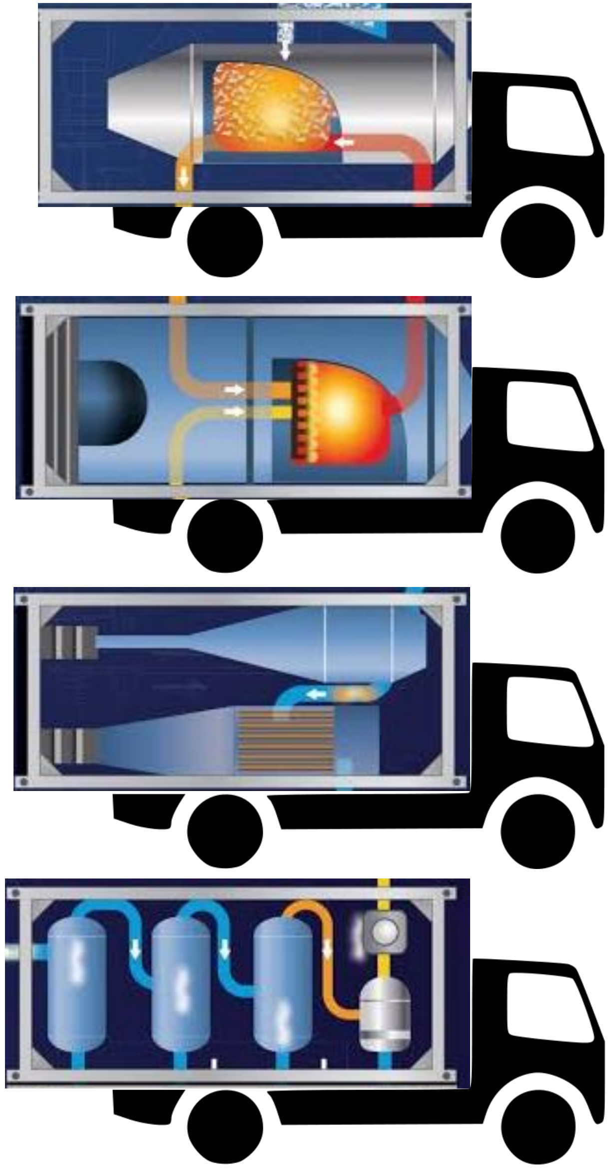
Waste Plastic Pyrolysis

Benefits of modular design:

Easy & efficient to set up new plants
→ network of local plants
→ minimise transport costs

Affordable & accessible to developing countries
Implementable with little infrastructure
→ Address plastic waste crisis where need is most pressing

Modular design minimises transport.



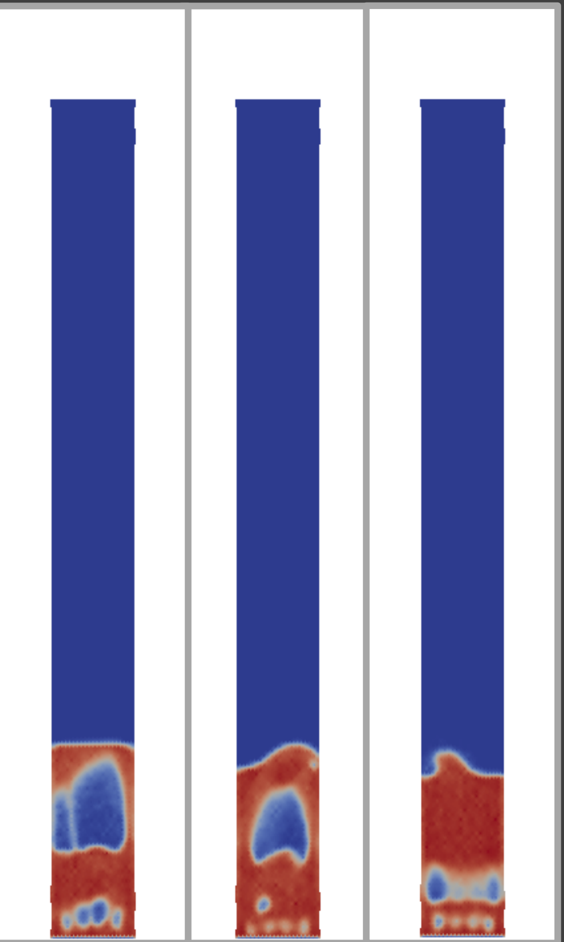
So what's the problem?

- Proven concept → commercial reality
- Reactor hydrodynamics **not fully understood**
- Improved knowledge needed for optimisation
- Large, opaque systems – how can we improve knowledge?

So what's the solution?

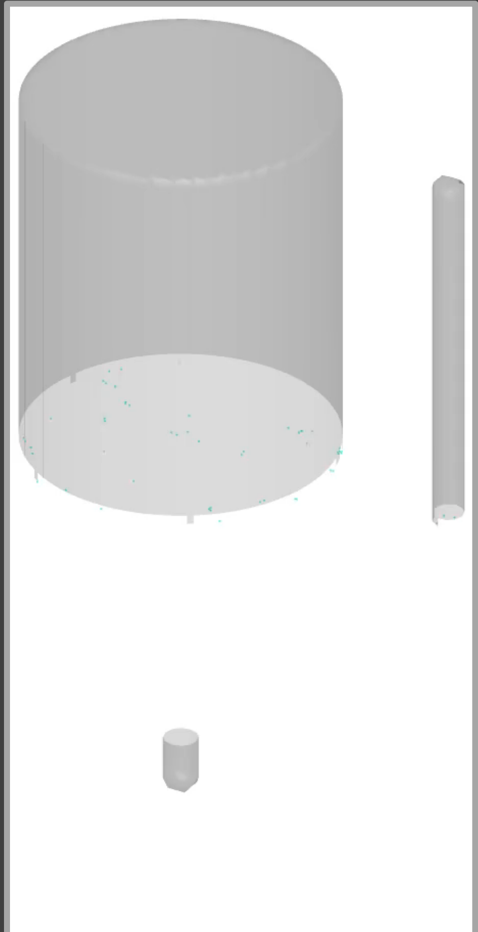
- Numerical modelling techniques capable of accurately predicting flow dynamics of large, multiphase systems
- Several main options for gas-solid systems:
  - CFD-DEM
  - MP-PIC
  - TFM

CFD-DEM (OpenFOAM-LIGGGHTS) vs. MP-PIC (Barracuda)



- Particles modelled as individual solid objects (DEM)
- Individual particle collisions **directly simulated**
- All physical parameters, including friction and restitution, directly implemented
- Comparatively slow (generally limited to order of 1M particles)

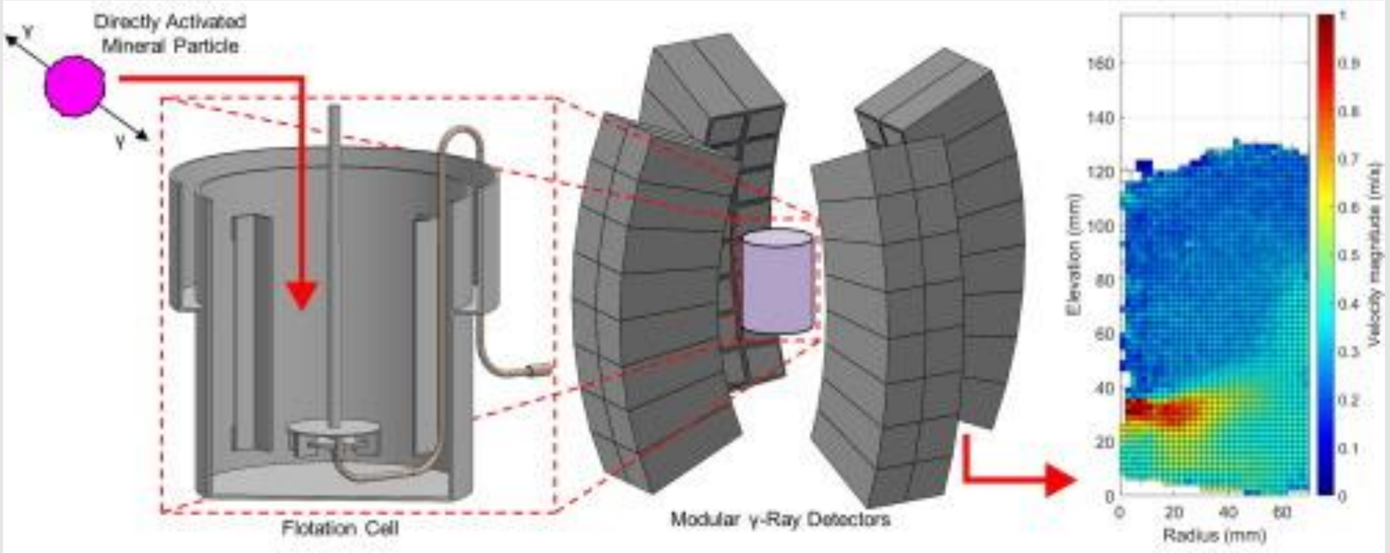
- Particles typically modelled in groups or “clouds”
- Interactions between clouds of particles **modelled**
- Friction and restitution indirectly modeled via normal stress, BGK collisions, and similar statistical models
- Comparatively fast (can simulate >100M particles)



Can either method faithfully reproduce dynamics of real fluidised-bed systems?

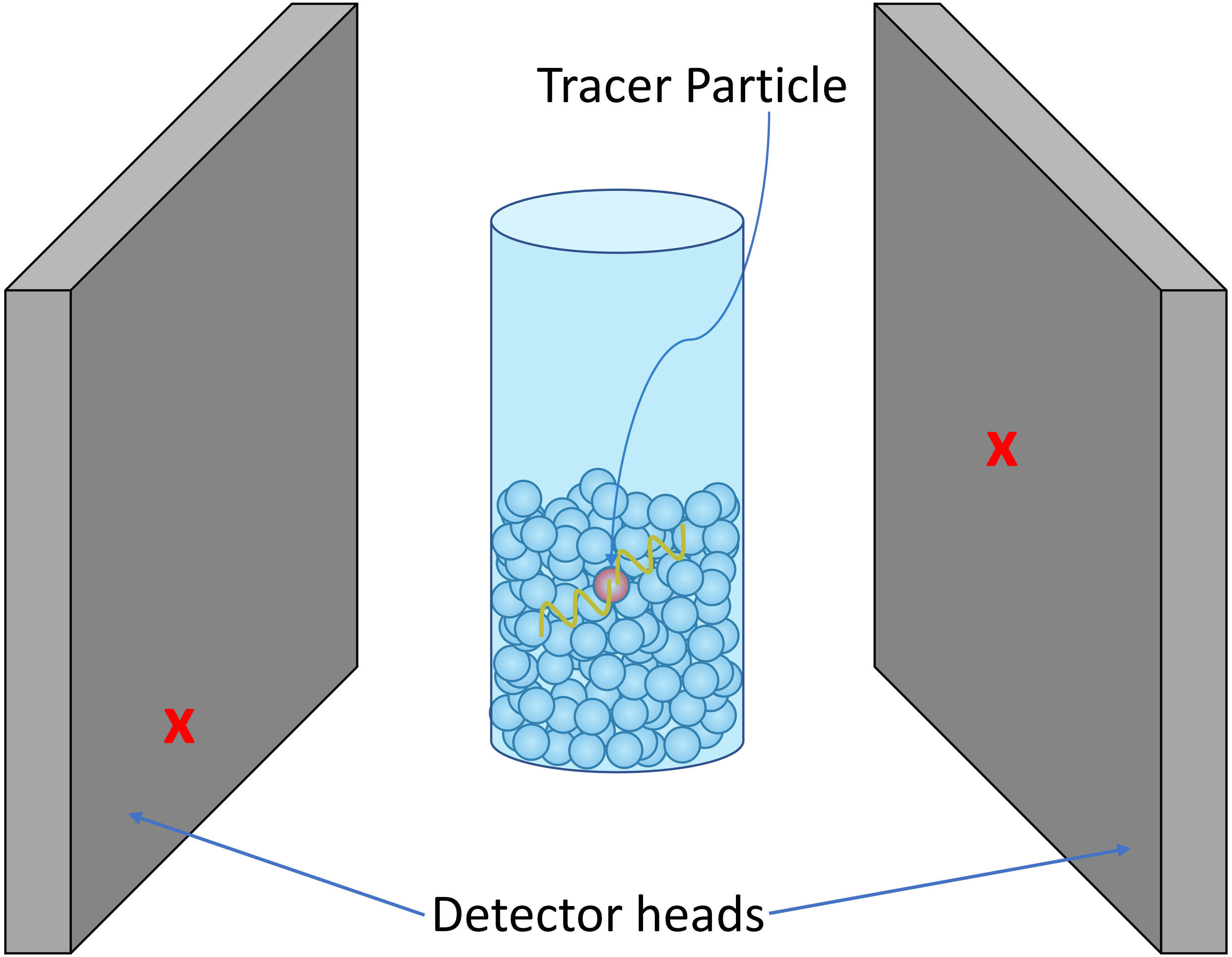
How can we rigorously test this?

Positron Emission Particle Tracking



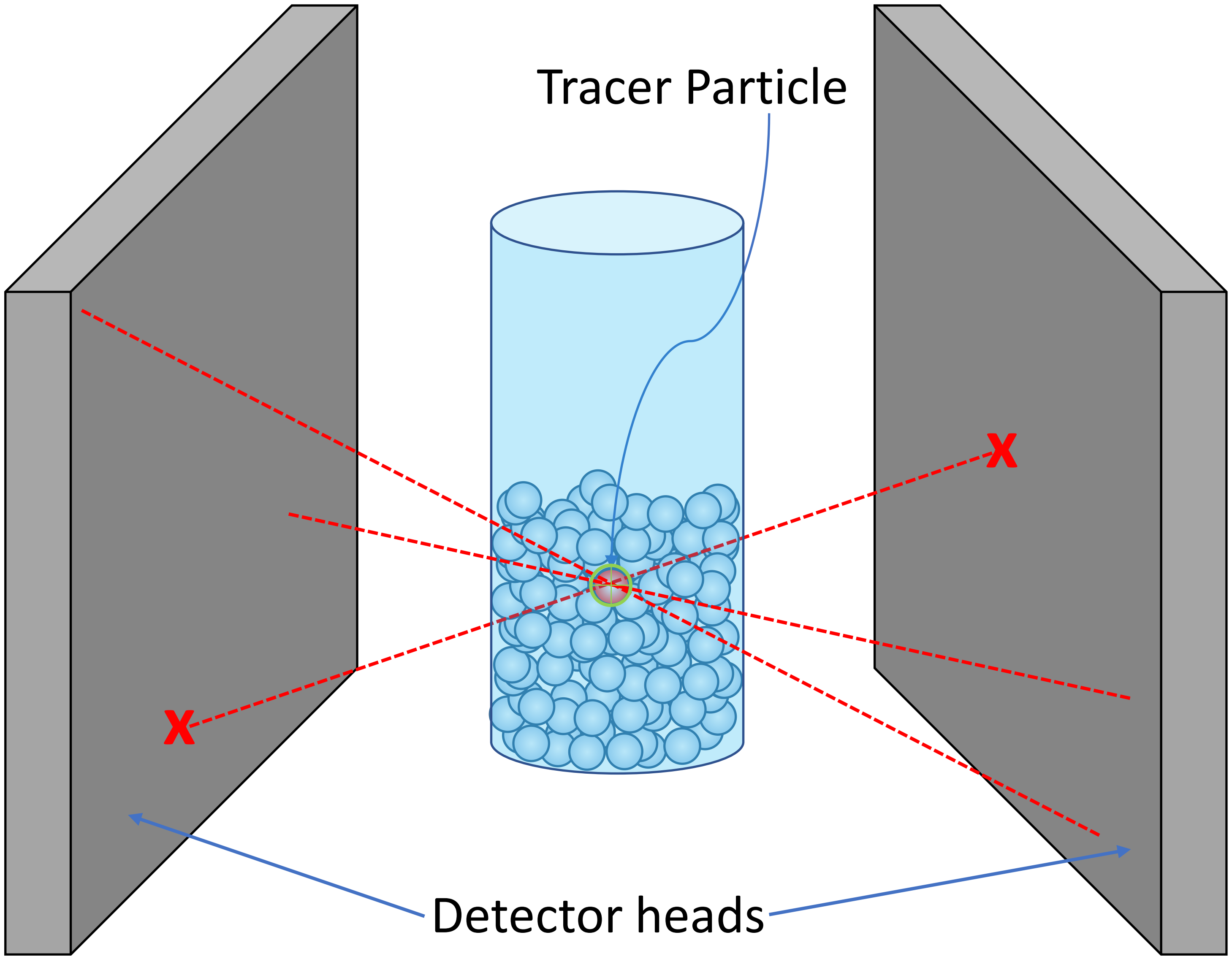
- Uses highly-penetrating gamma radiation to directly track the three-dimensional motion of particles through particulate, fluid and multiphase systems, with high temporal and spatial resolution.
- PEPT is **uniquely well suited** to validation of numerical models
  - Detailed, 3D images of dynamics → direct, quantitative comparison with numerical data
  - Can "see inside" steel-walled industrial systems

Positron Emission Particle Tracking



Windows-Yule, C. R. K., Seville, J. P. K., Ingram, A., & Parker, D. J. (2020). Positron Emission Particle Tracking of Granular Flows. *Annual Review of Chemical and Biomolecular Engineering*, *11*.

Positron Emission Particle Tracking



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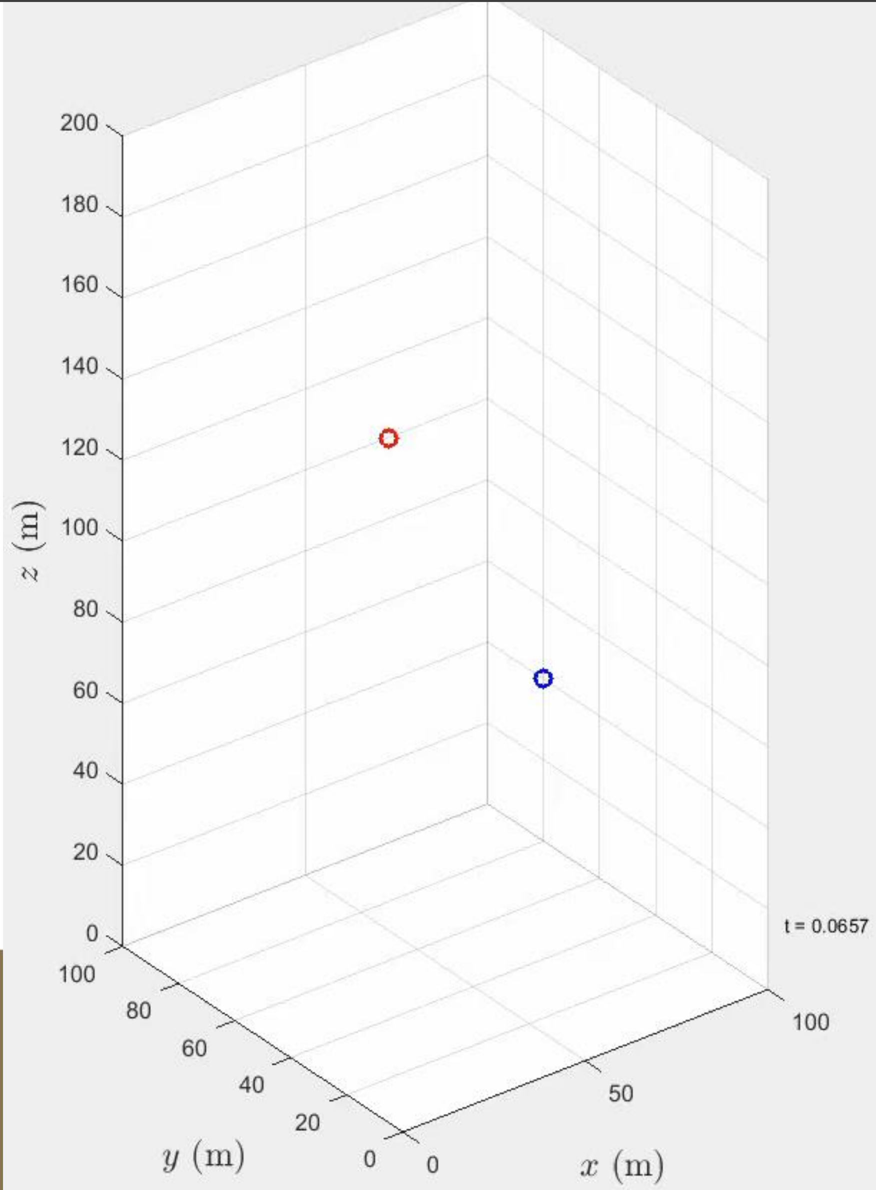
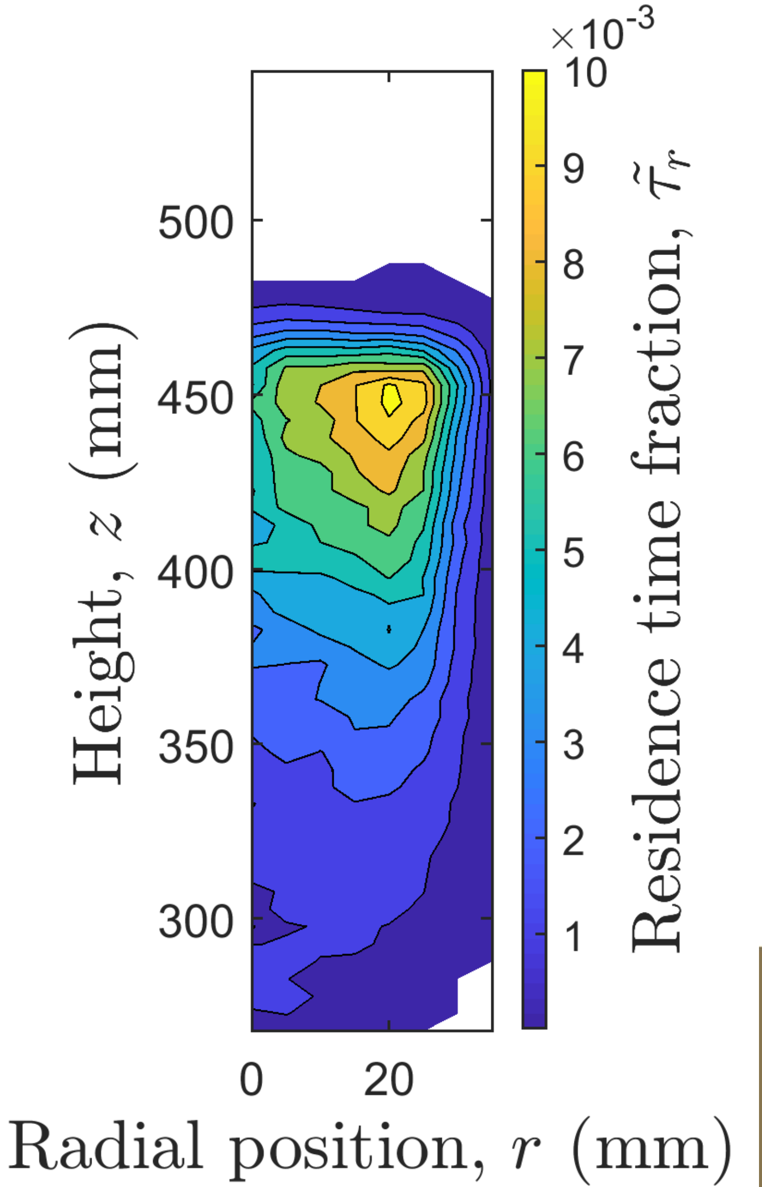
Validation: Positron Emission Particle Tracking



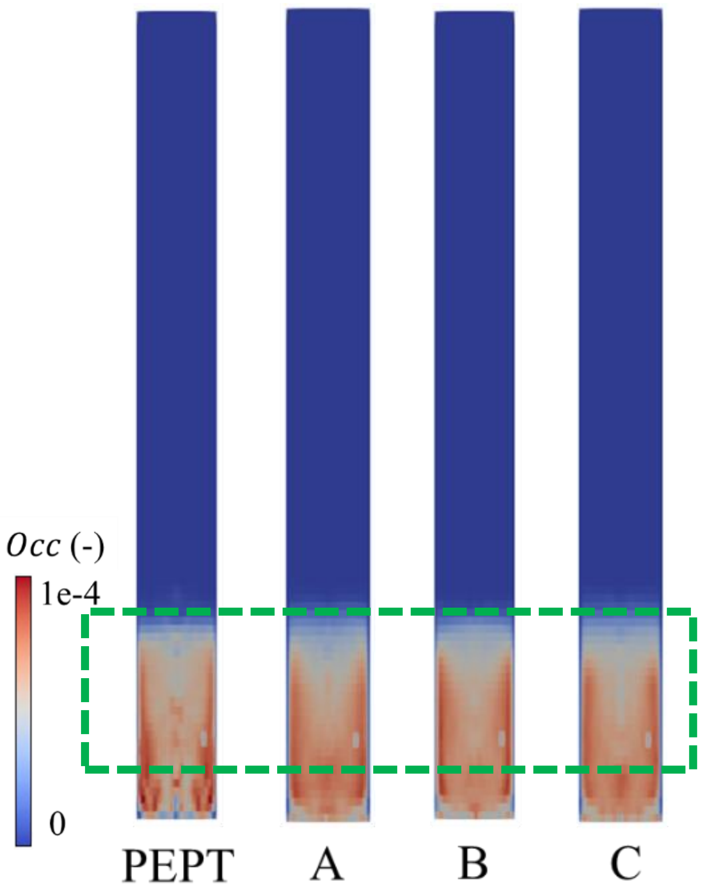


Validation

- PEPT experiments conducted in 2 fluidised beds, 100 mm and 200 mm inner diameter
- Range of fluidisation velocities (U) and fill heights (H)
- Material: 300 micron sand identical to that used in plastic recycling process

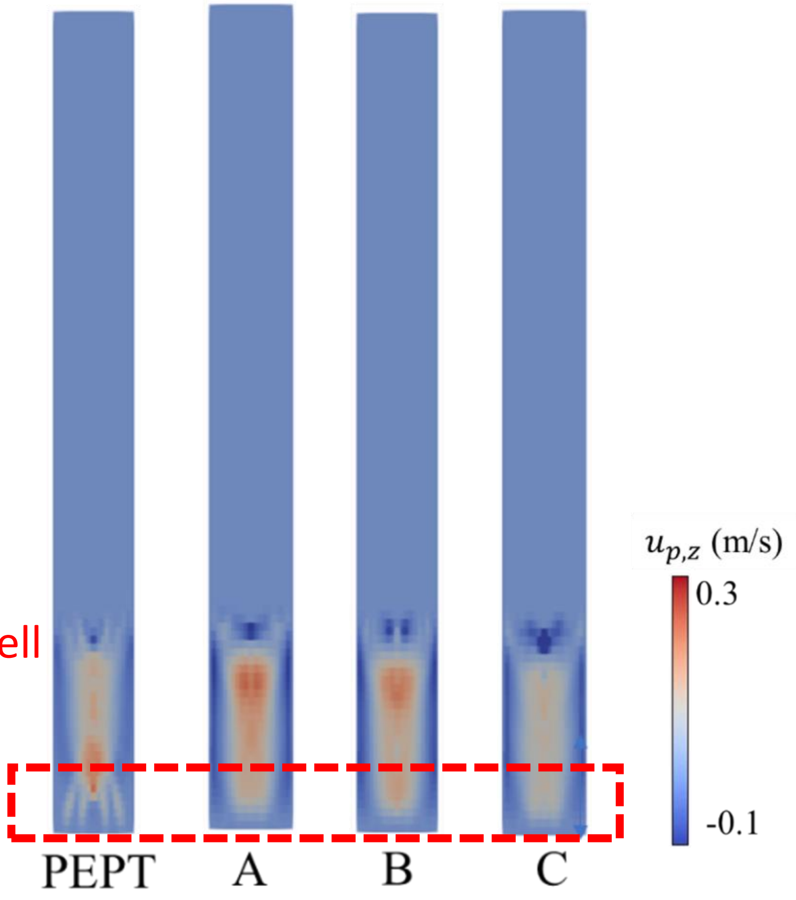
Validation: CFD-DEM vs. PEPT

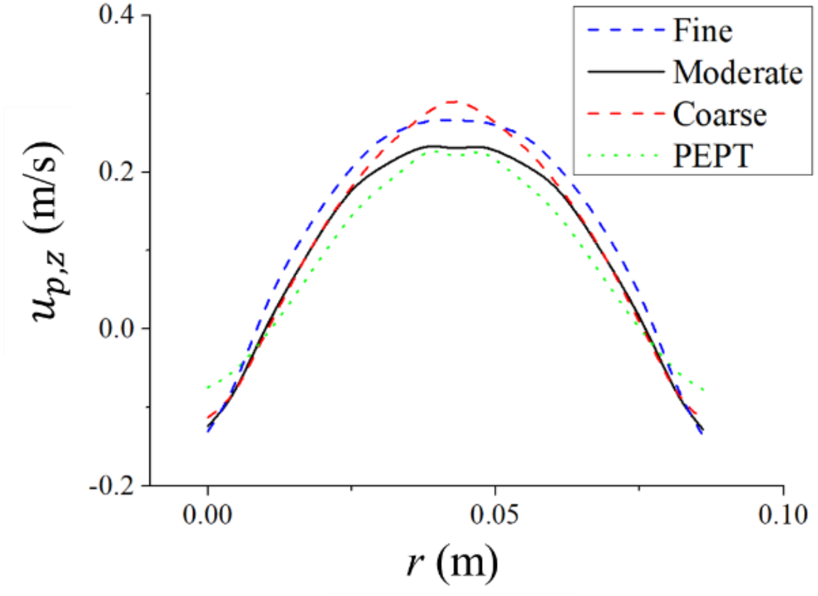
100 mm Case

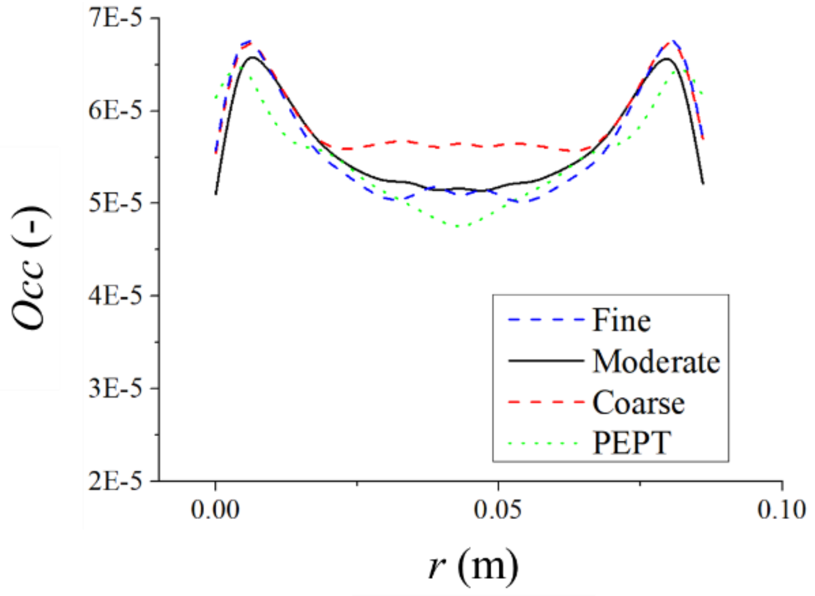


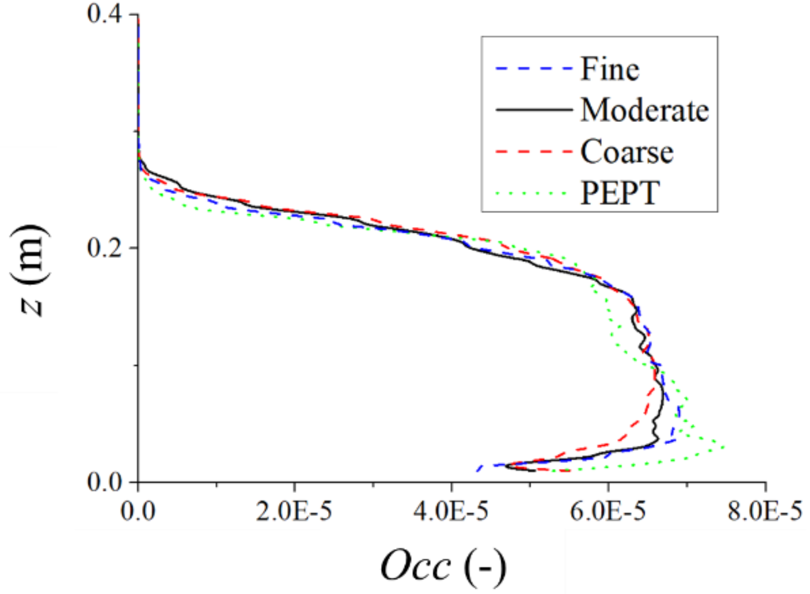
Remainder of bed more faithfully reproduced

Distributor region not well captured



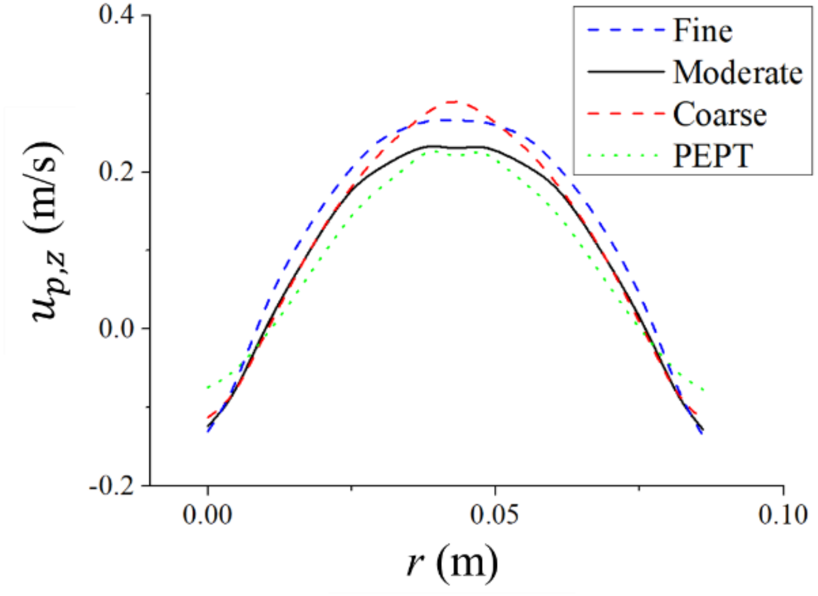


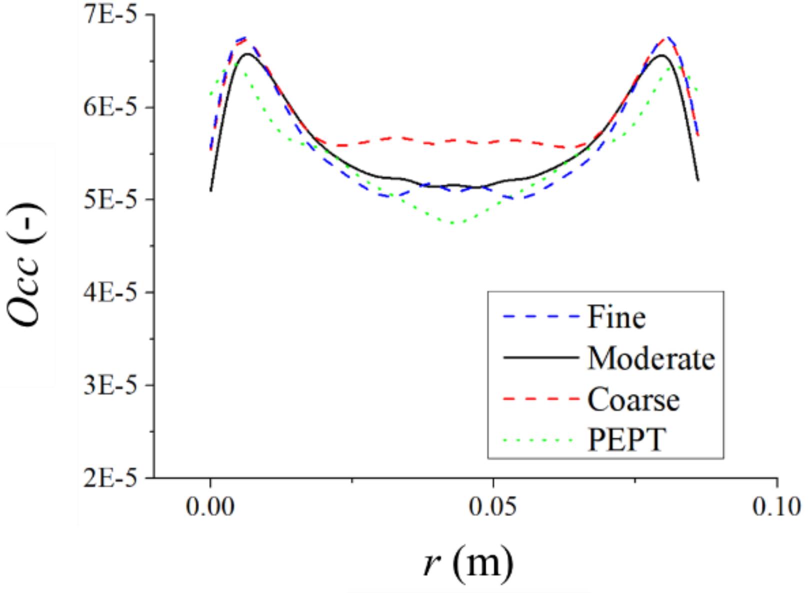


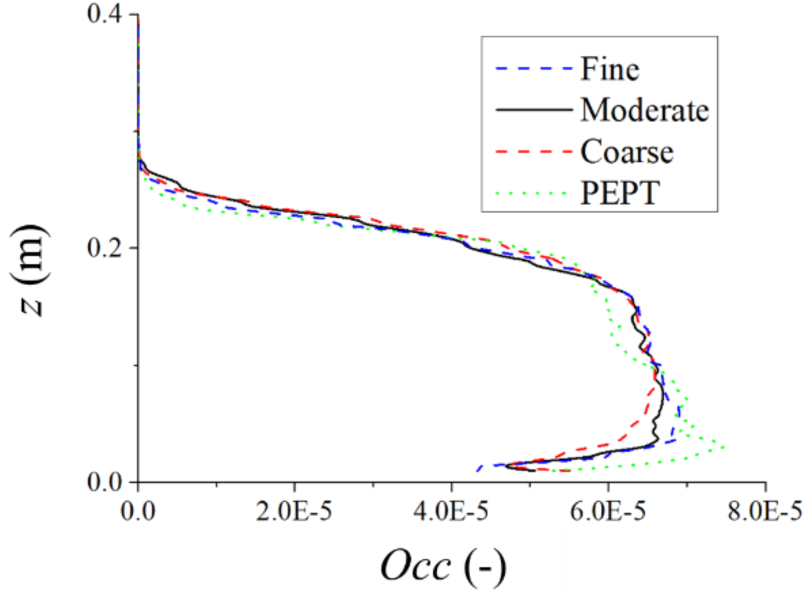


Validation: CFD-DEM vs. PEPT

Neglecting immediate vicinity of distributor, good, quantitative, mesh-invariant agreement with PEPT data





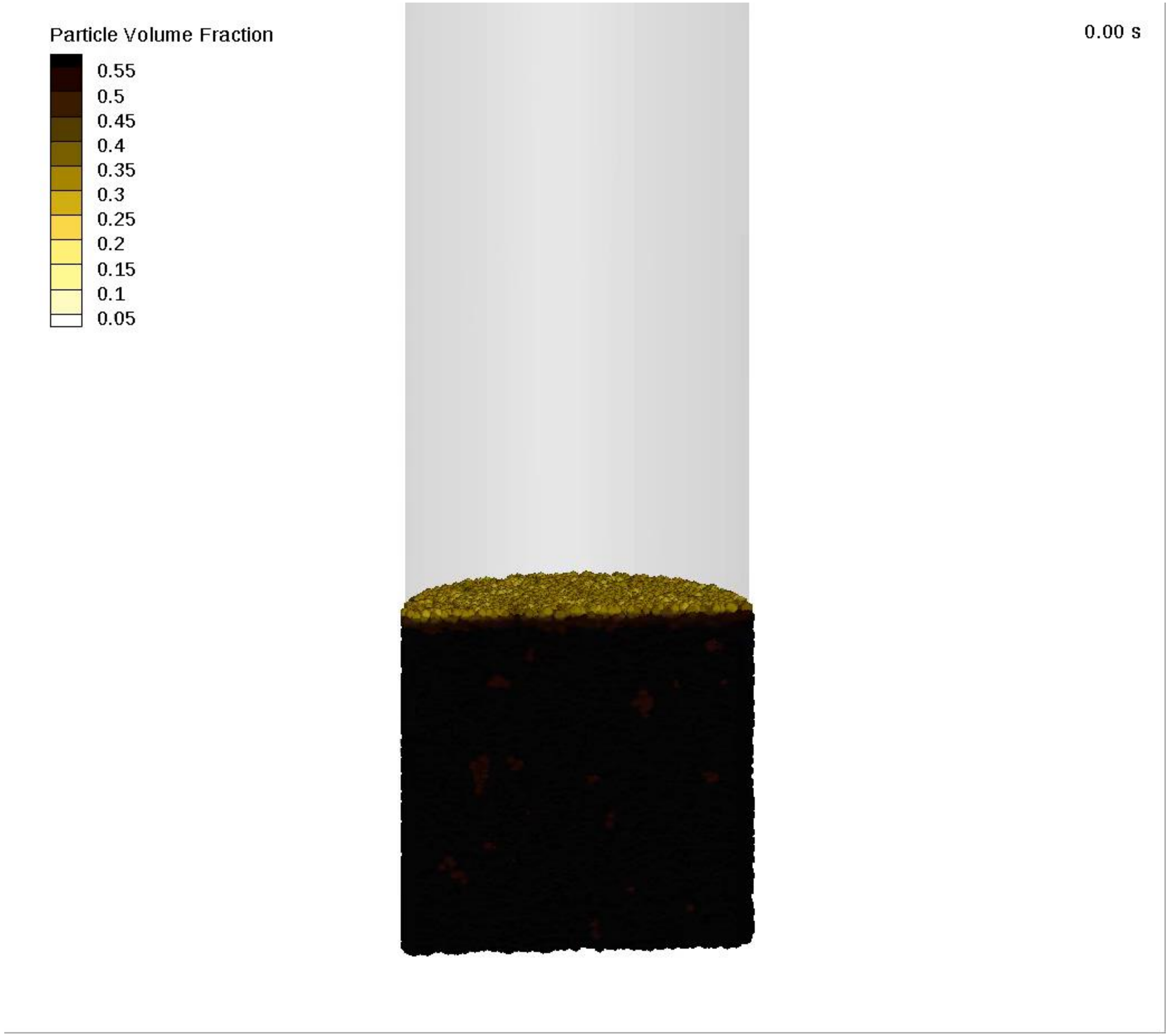


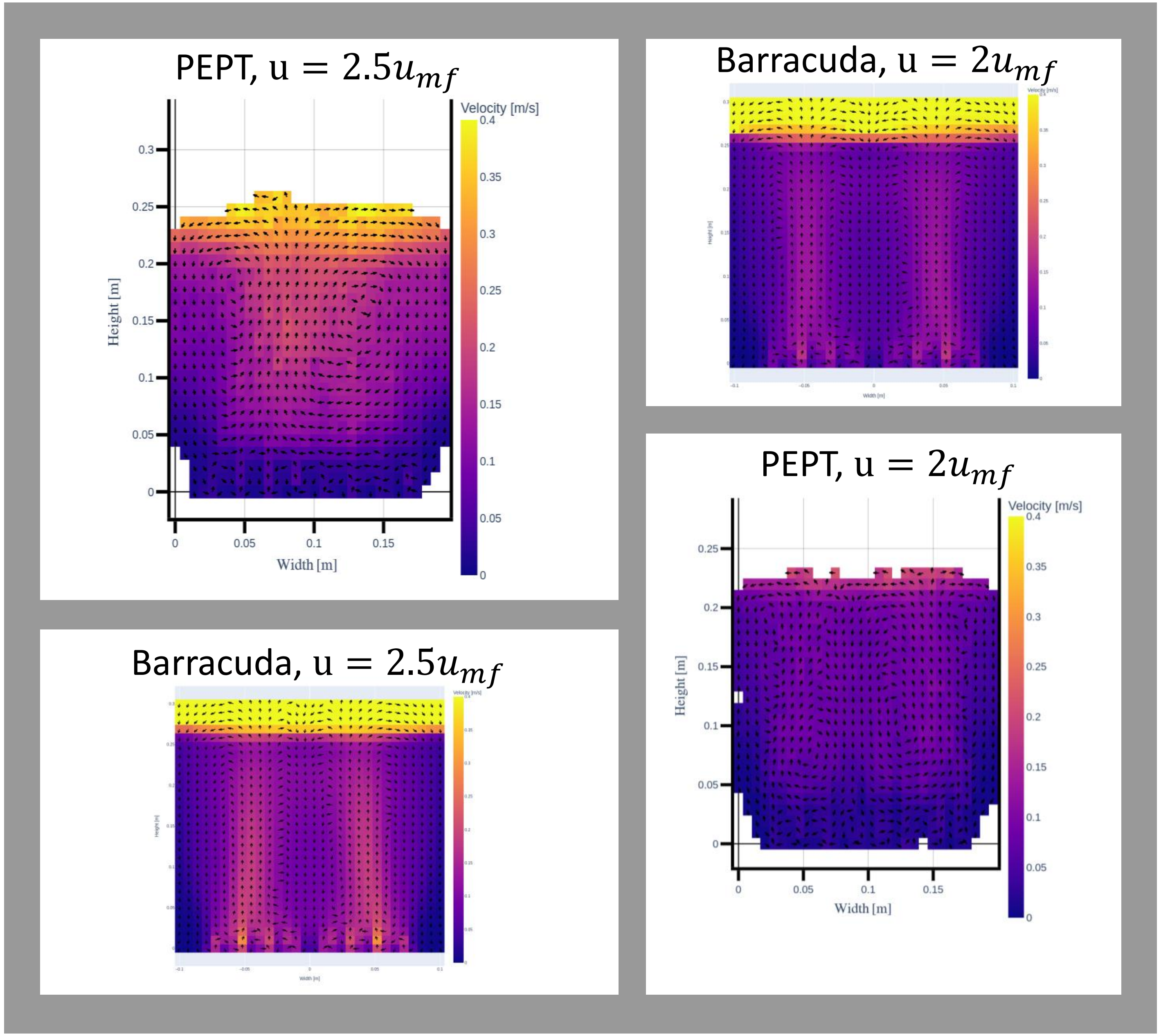
Validation: CFD-DEM vs. PEPT

For 200 mm case, however, large N ($\sim O(100\text{M})$) renders problem intractable without significant coarse-graining

Validation: MP-PIC vs. PEPT

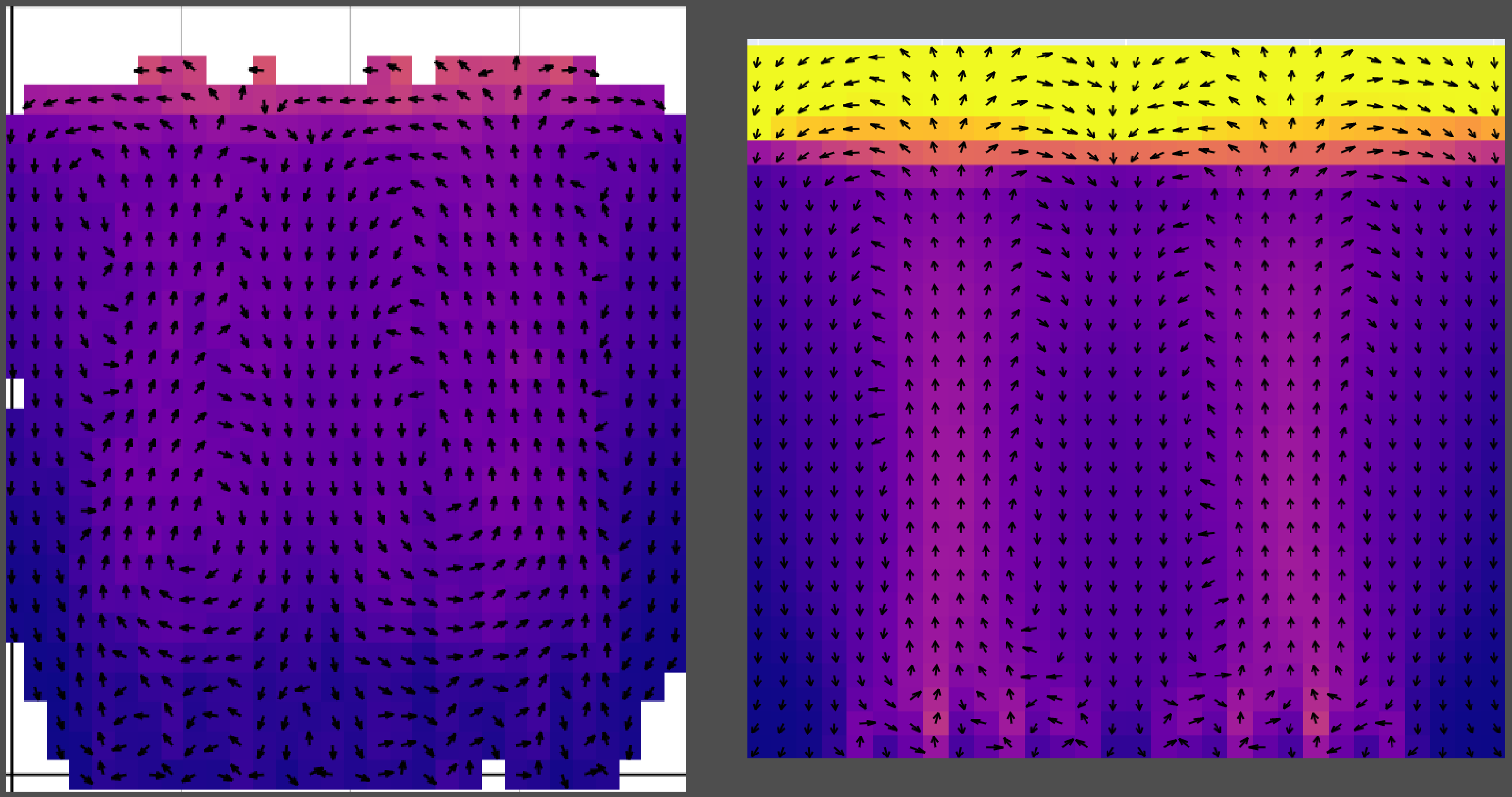
- For 100 mm rig, agreement not observed for wide parameter sweep
- Neither qualitative nor quantitative agreement for any parameters tested
- **But** better results for larger system

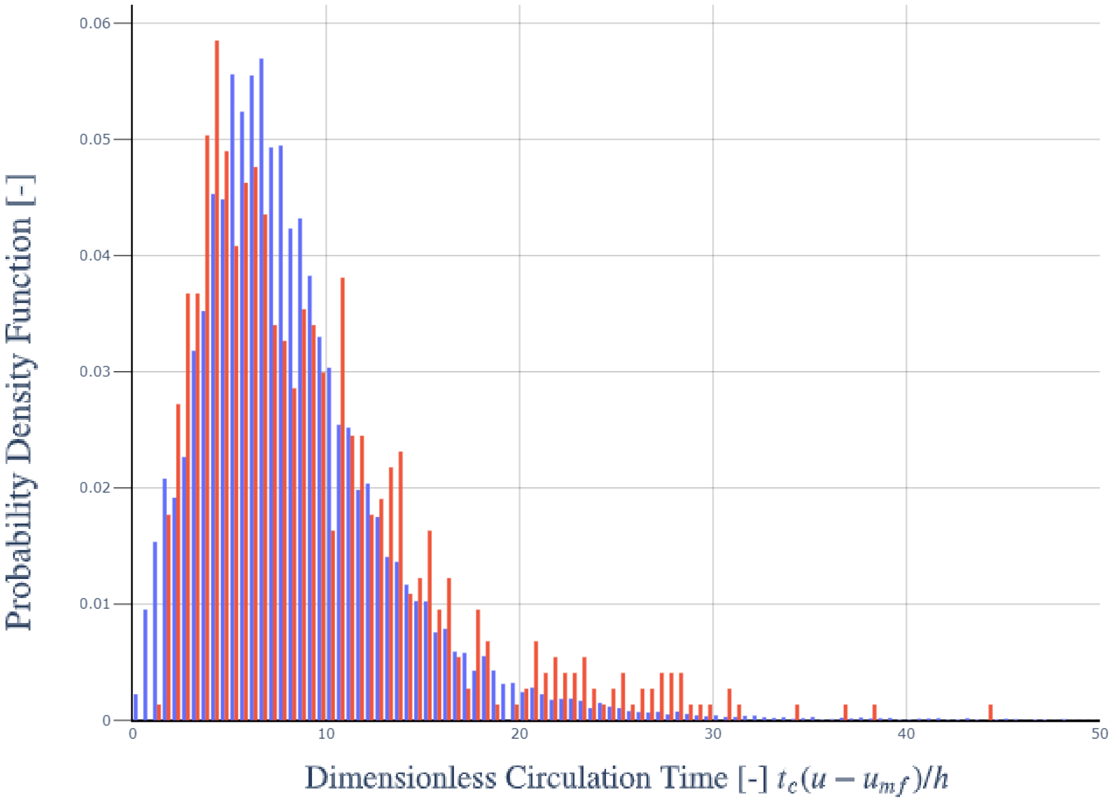


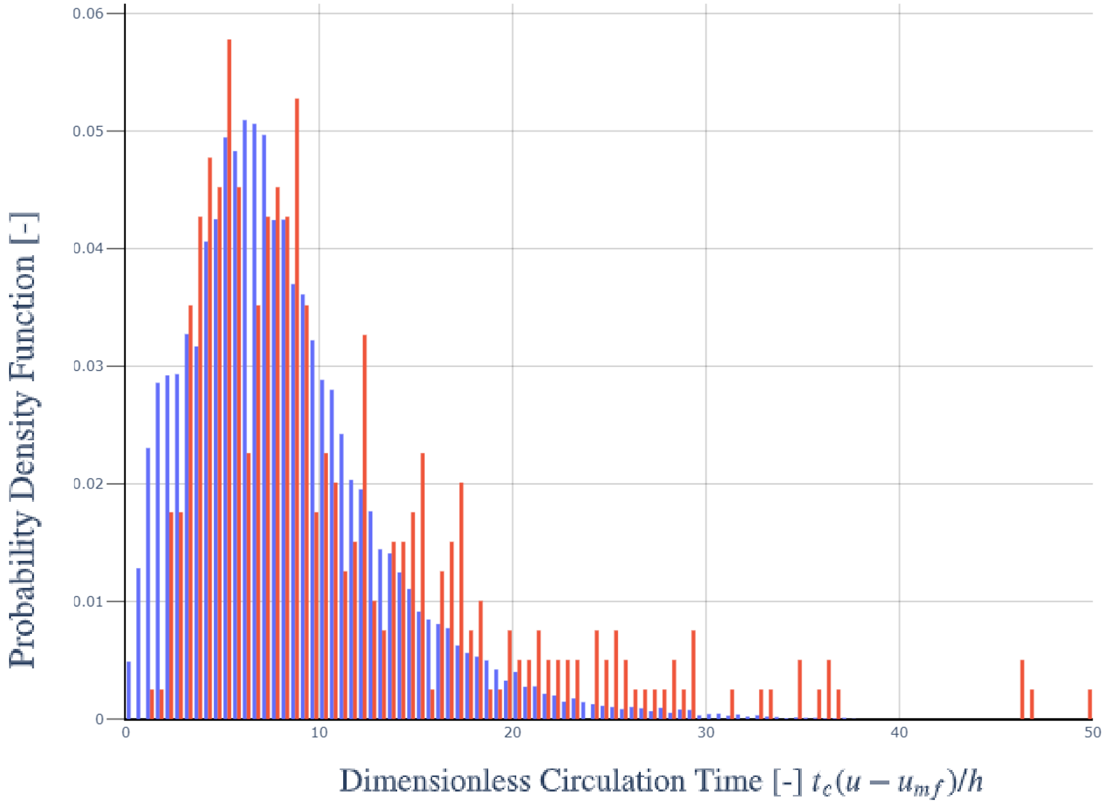


Validation: MP-PIC vs. PEPT

- Reasonable agreement between measured and predicted expanded bed heights
- Similar ranges of velocities between experiment and simulation
- Qualitatively matching flow patterns for lower u, some deviation at higher u



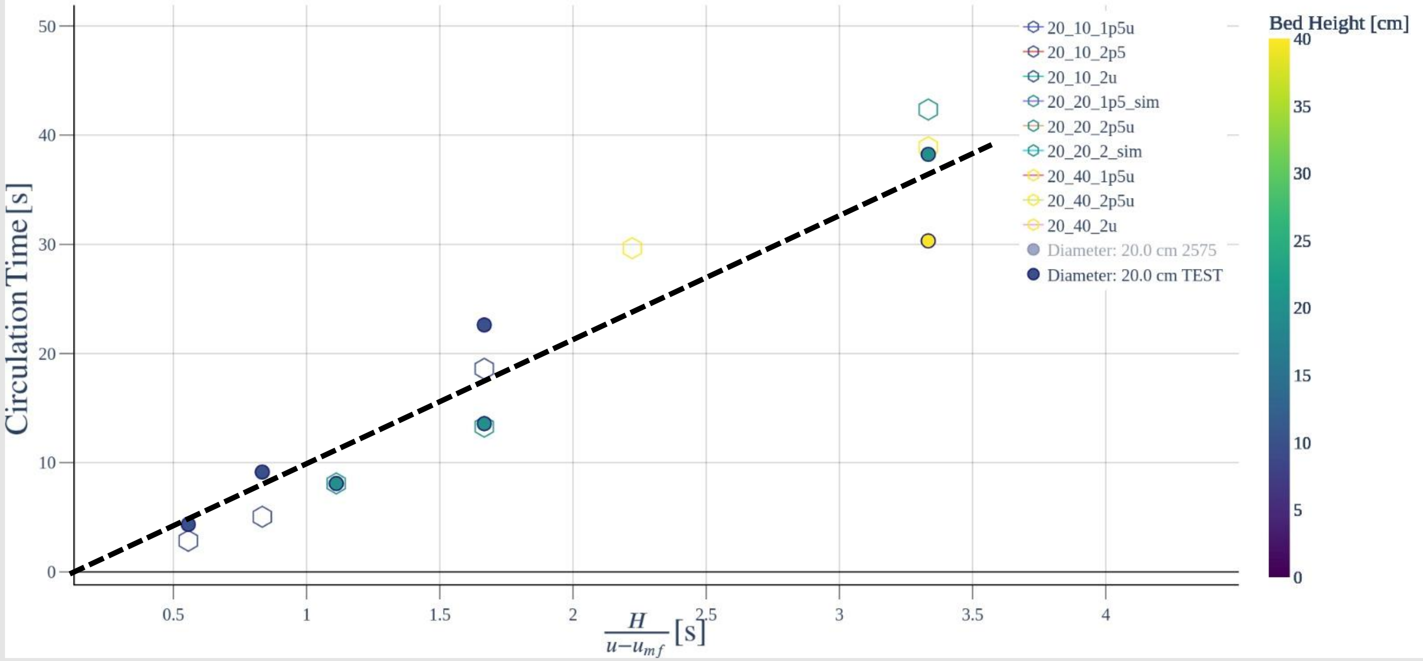




Circulation Rate

PEPT || MP-PIC

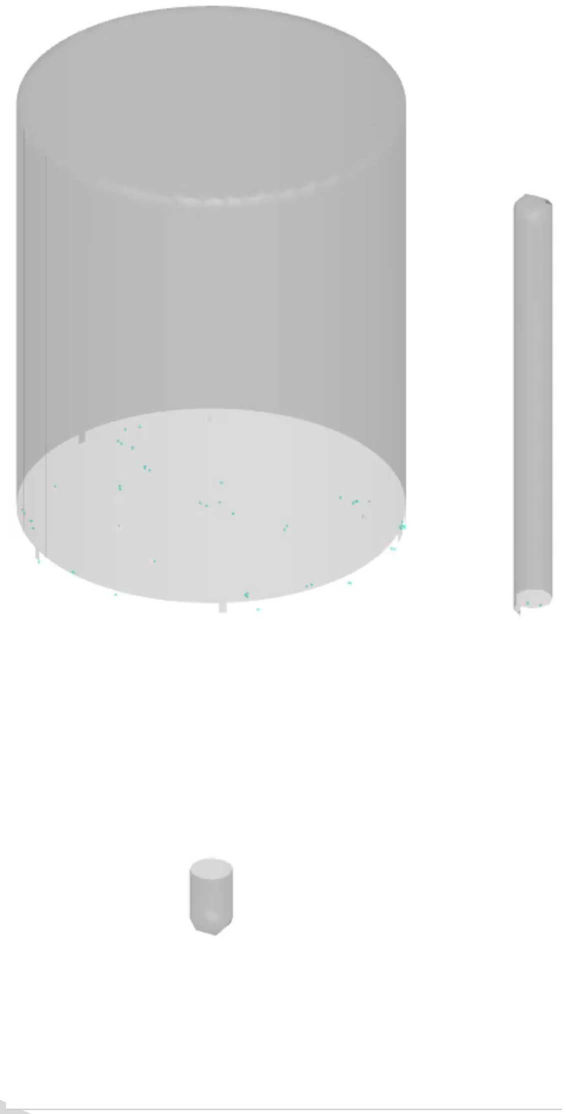
Circulation Rate



- Barracuda data scales with $\frac{H}{u-u_{mf}}$ as expected from the literature
  - → Results are **physical**
- Close correspondence between PEPT and Barracuda
  - → Results are **accurate**
- Disagreement largely due to **lack of statistics from experimental data**

Summary

- CFD-DEM and MP-PIC simulations validated against PEPT data
- CFD-DEM capable of providing quantitative accuracy at small scales, but unfeasible for larger systems
- MP-PIC unsuitable for narrow vessels, likely due to limited statistics (not enough particles per cell)
- Take-home point:
  - CFD-DEM for precise, lab-scale simulations
  - MP-PIC for pilot and industrial simulations



Any and all questions are very welcome