Small Scale Experimental and Modeling Studies for Geldart Group A Particles

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Outline

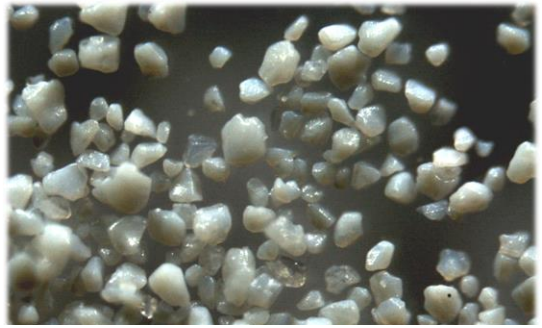
- Challenges in modeling Group A particles
- Mini-C2U with MFIX-TFM simulations
- Pseudo-2D bed with MFIX-DEM simulations
- Drag evaluation for different flow regimes
- Concluding remarks

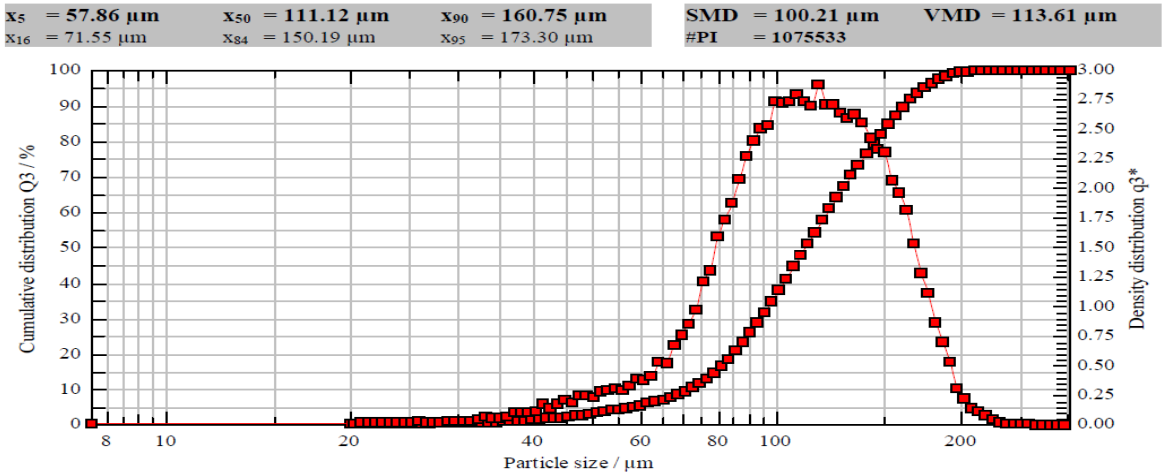
Challenges in Modeling Group A Particles

- **Group A particles**
  - Large surface area, good fluidization properties
  - Widely utilized in various industrial processes, e.g. FCC
- **Challenges in CFD modeling**
  - TFM
    - Over-prediction of bed expansion using TFM were widely reported in the literature
    - Effects of cohesive force and PSD are important but hard to consider in TFM
    - Good heterogeneous drag models such as EMMS drag are needed for Group A particles
  - DEM
    - Very expensive to simulate due to the large particle count encountered in most applications
    - Lack of small-scale experiment with manageable particle count and detailed measurements for validation

Mini-C2U for CO2 Sorbents

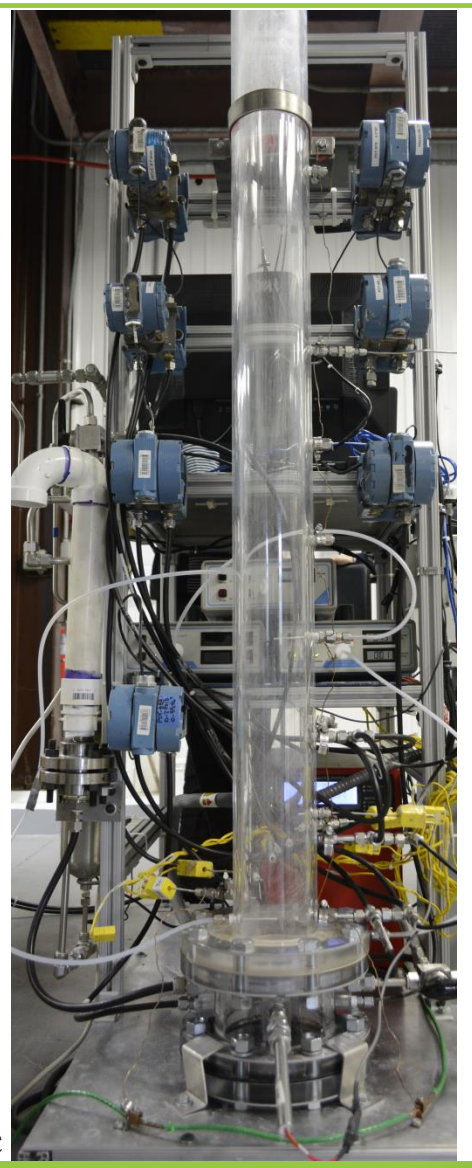
- **10-cm bubbling bed (Li et al. 2016)**
  - NETL 32D sorbents
    - Diameter: 100 μm
    - Density: 480 kg/m3
    - Umf: 0.0023 m/s

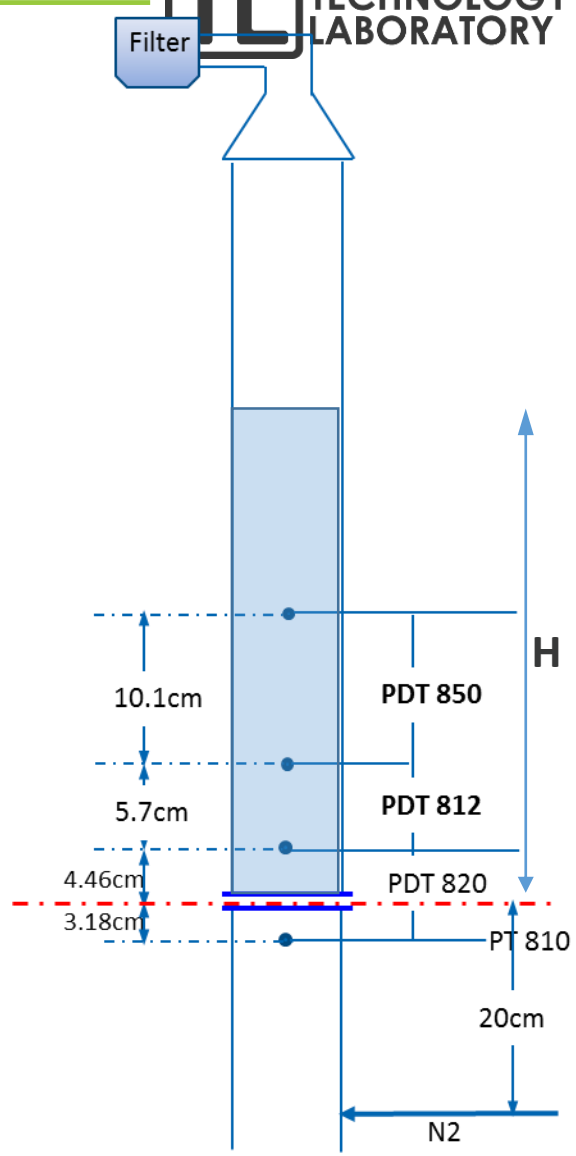




  - Objectives
    - In support of CCSI project
    - **Flow hydrodynamics** and CO2 capture performance

CCSI
Carbon Capture Simulation Initiative

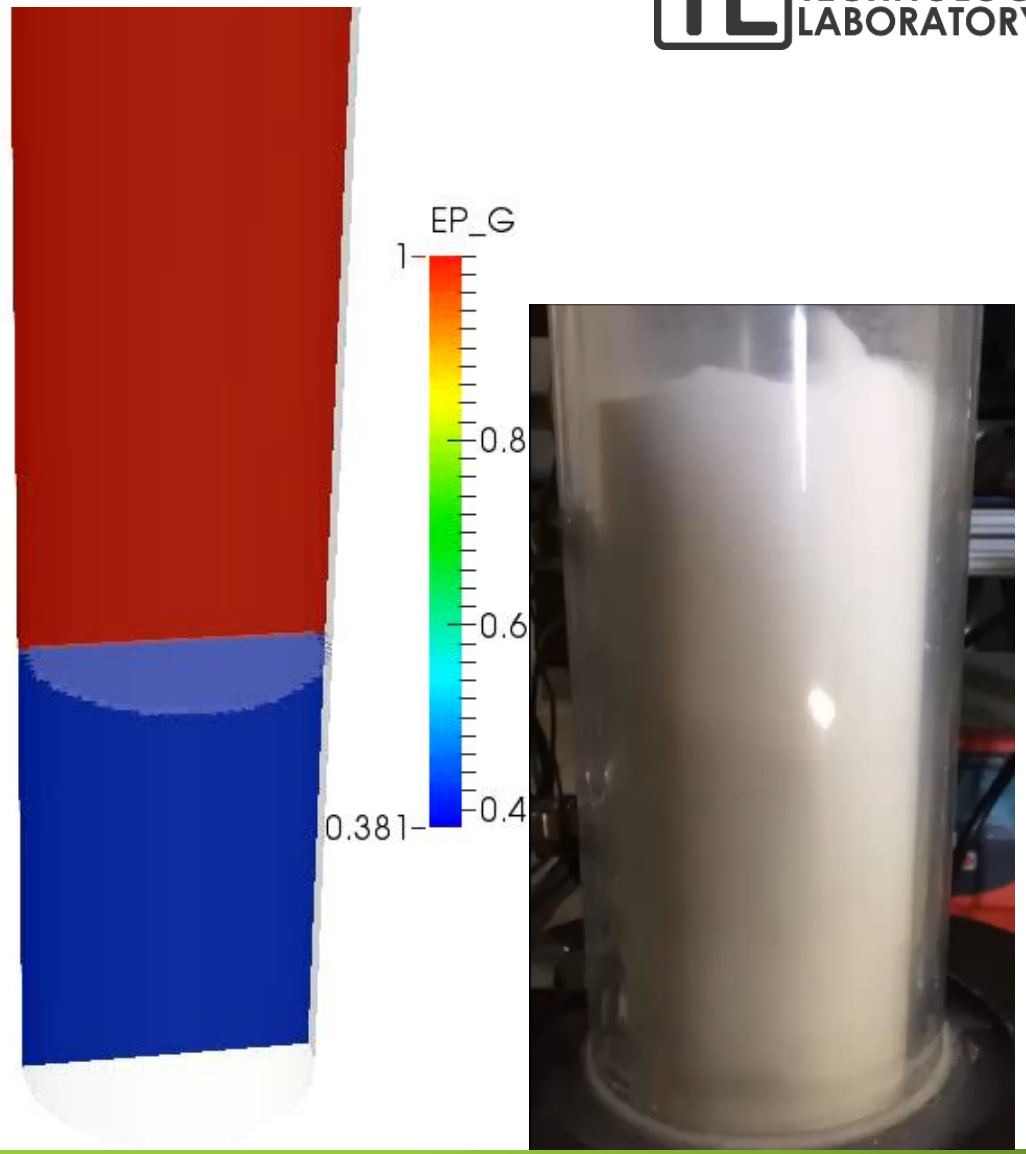




Experimental setup and schematic for measurements

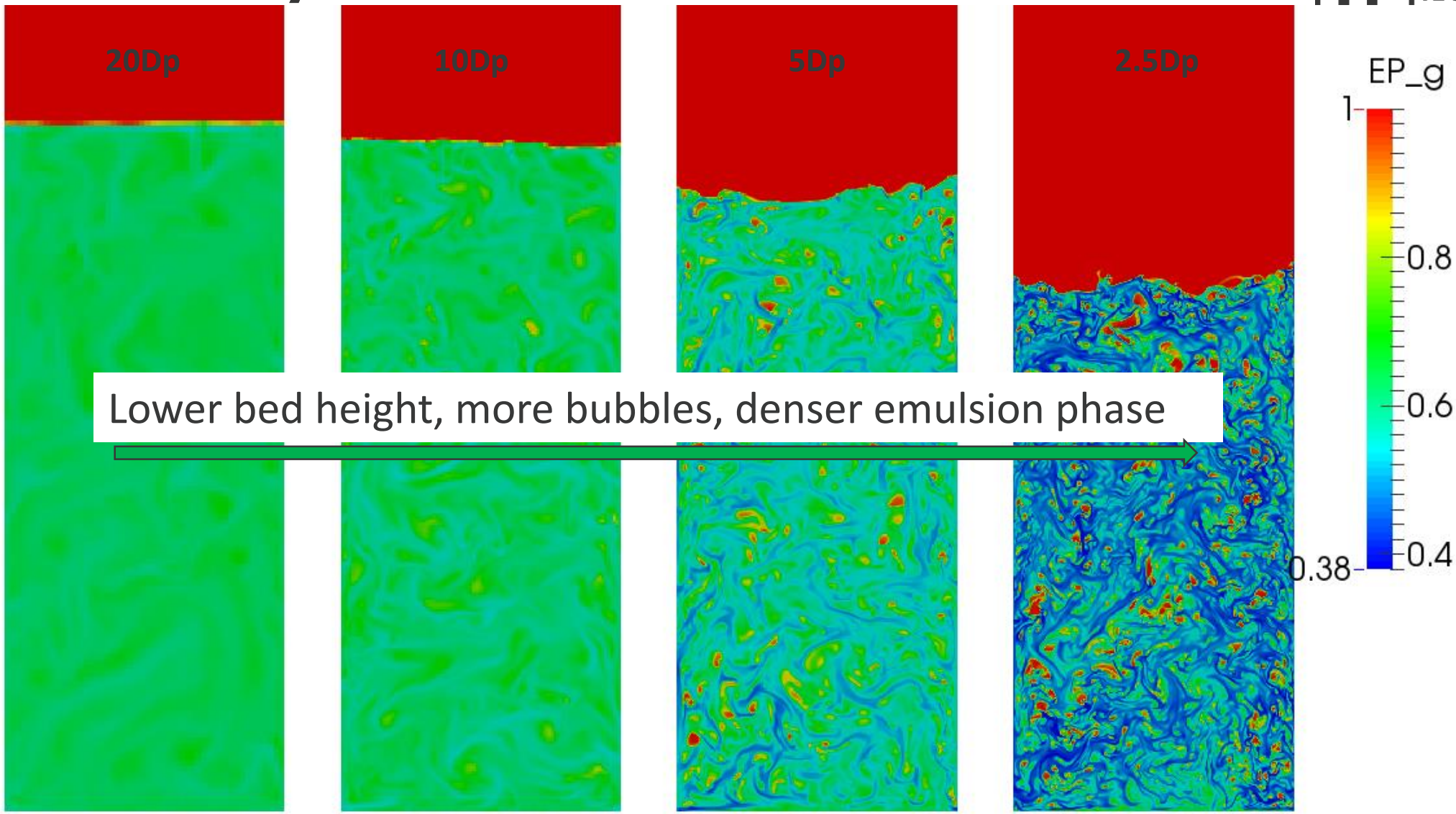
Numerical Simulation

- **Flow conditions**
  - Static bed height: 15cm
  - Superficial velocity: 5 Umf
- **Numerical model**
  - MFIX-TFM with kinetic granular theory
  - Algebraic granular temperature
  - Schaeffer friction model
  - Grid size: 4 mm = 40 Dp
- **Observation**
  - Homogeneous expansion vs. vigorous bubbling
  - Over-prediction of bed height: 24 cm vs. 19 cm
  - Similar to literature results for Group A particles



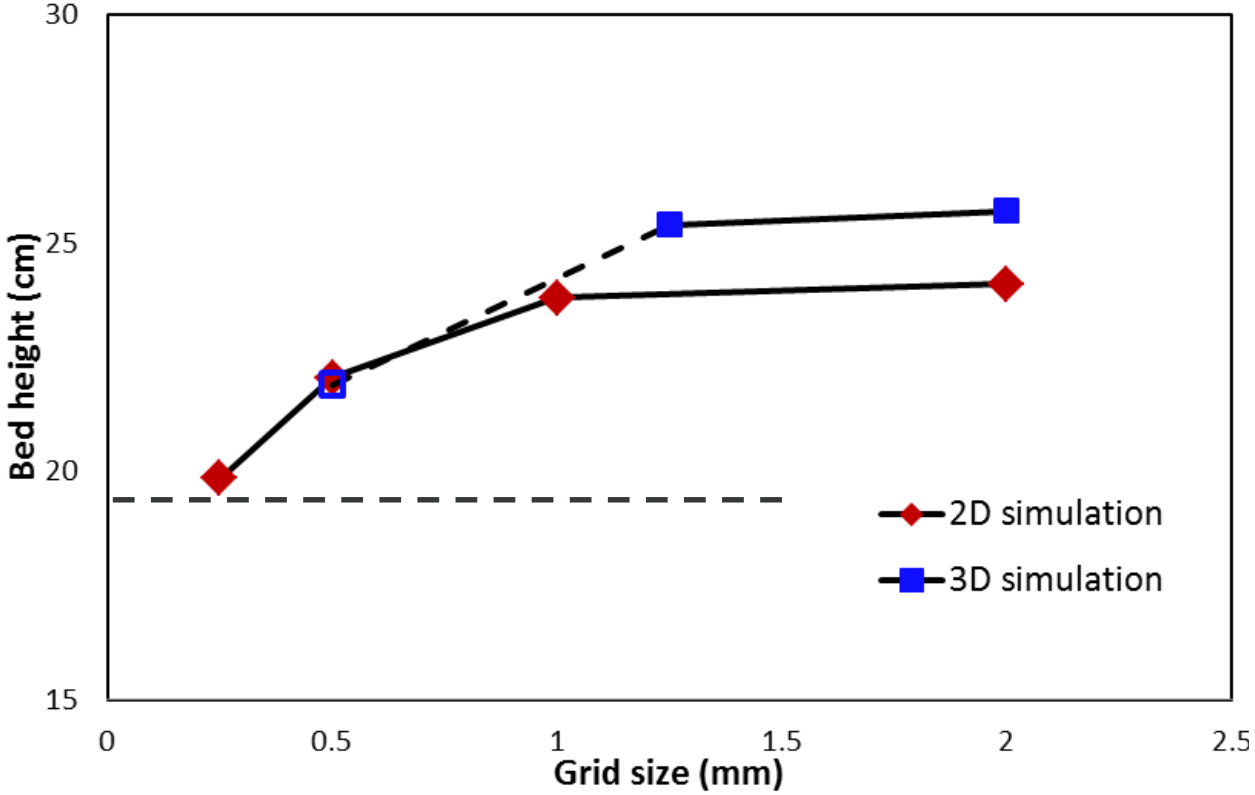
Simulation (left) and experiment (right) for 5Umf

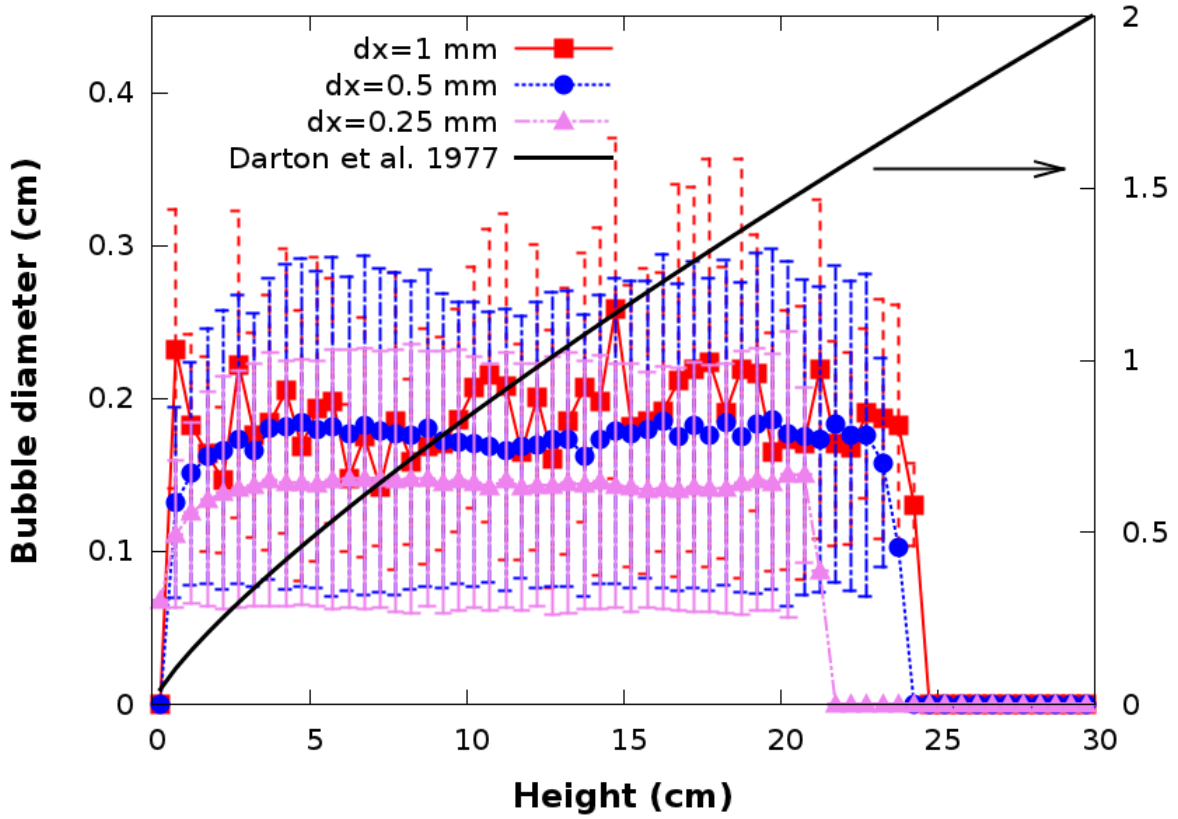
2D Grid Study



Numerical Results

- Bed height and bubble analyses

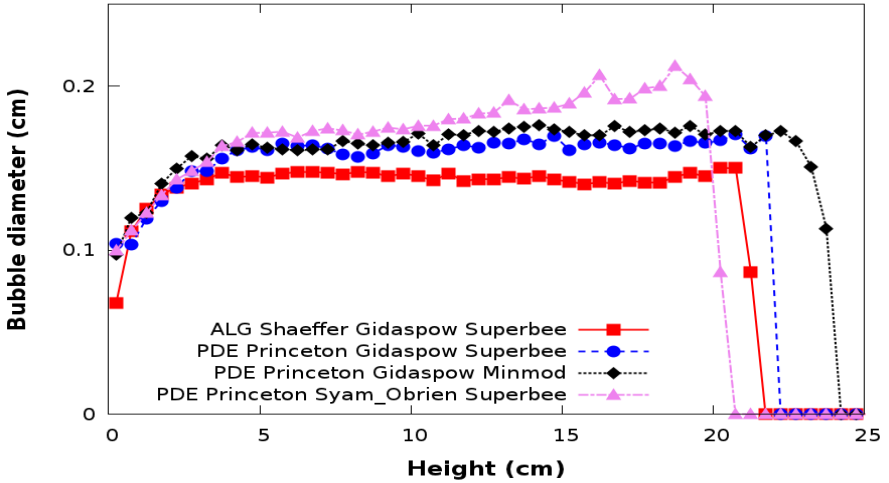


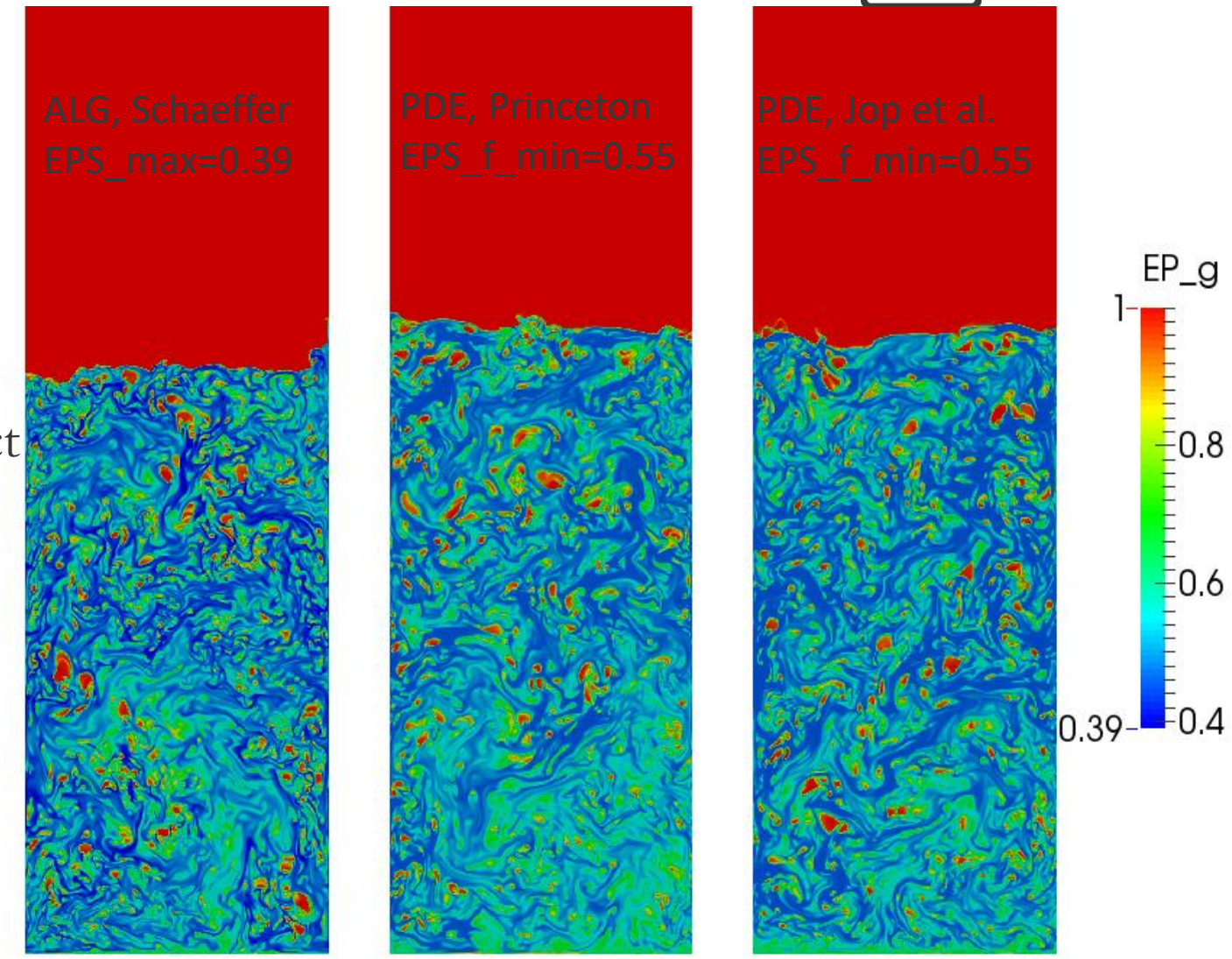


- Bed expansion height can be reasonably matched with the fine numerical grid
- Unrealistic small bubbles are predicted by 2D fine grid numerical simulations

Effect of Model Setting

- **Model setting**
  - ALG/PDE granular temperature
  - Different friction models
  - Fine grid: 2.5Dp
- **Observation**
  - Friction model has no strong impact
  - Many small bubbles in simulation





Snapshots of voidage distribution from 2D simulations

Filtered Model Simulation

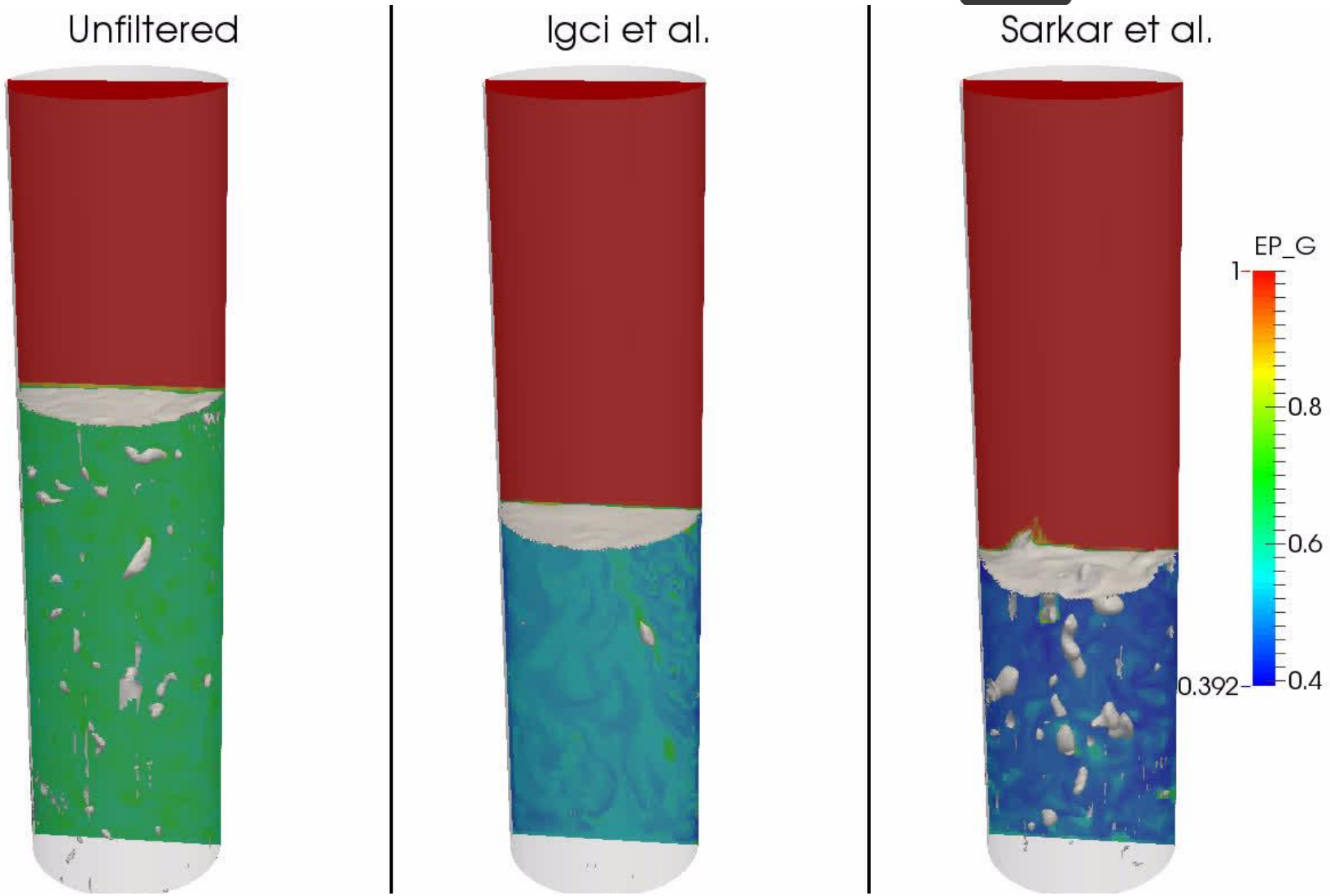
- **Model setting**
  - Filtered drag models
  - No filtered stress model
  - Grid size: 2mm=20Dp
- **Comparison**
  - Sarkar et al. drag results

Bed heights predicted by different drag models and experimental measurement.

Tests	Gidaspow	Igci et al.	Sarkar et al.	Exp.
Bed height (cm)	25.8	21.3	17.1	18.7

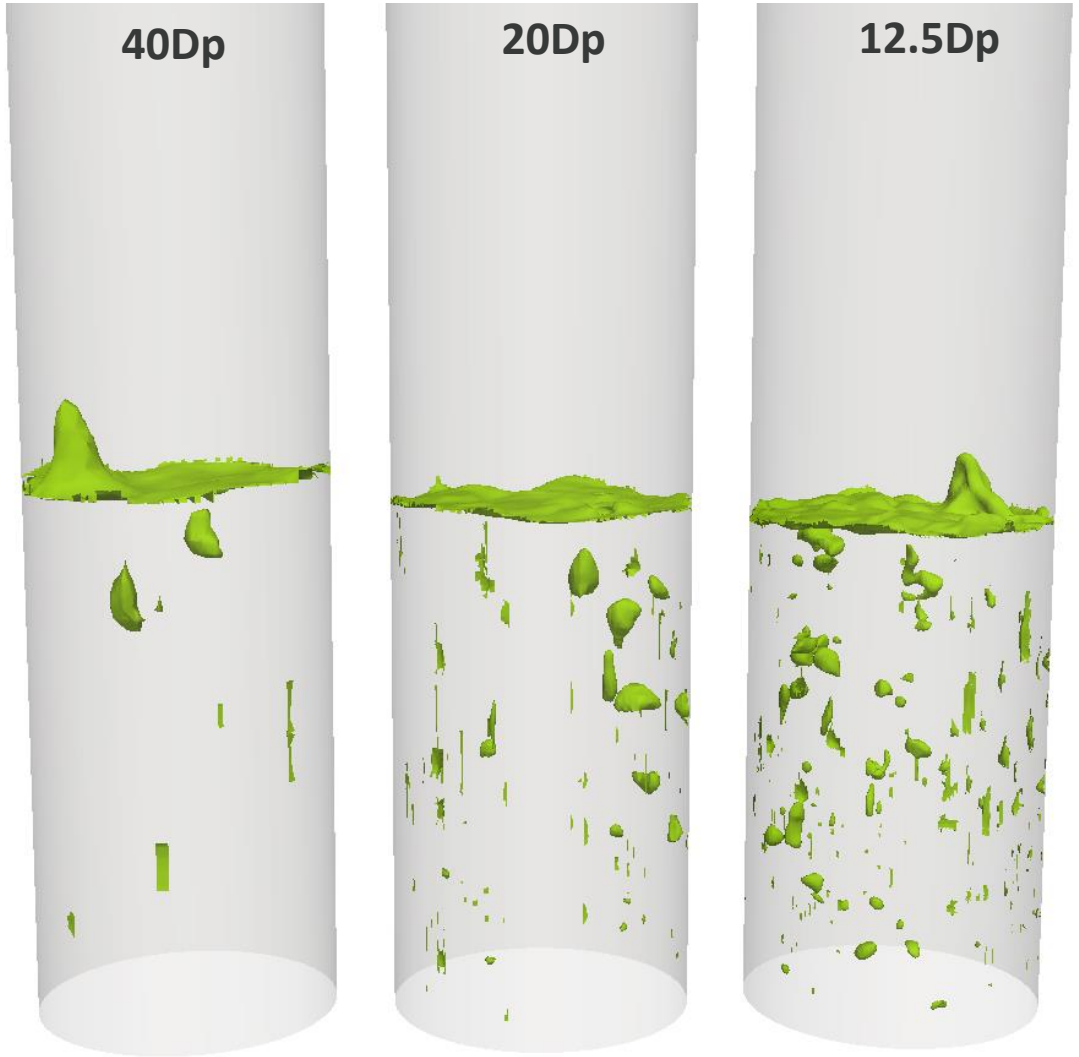
Numerical predictions and experimental measurement of pressure drop for different tests.

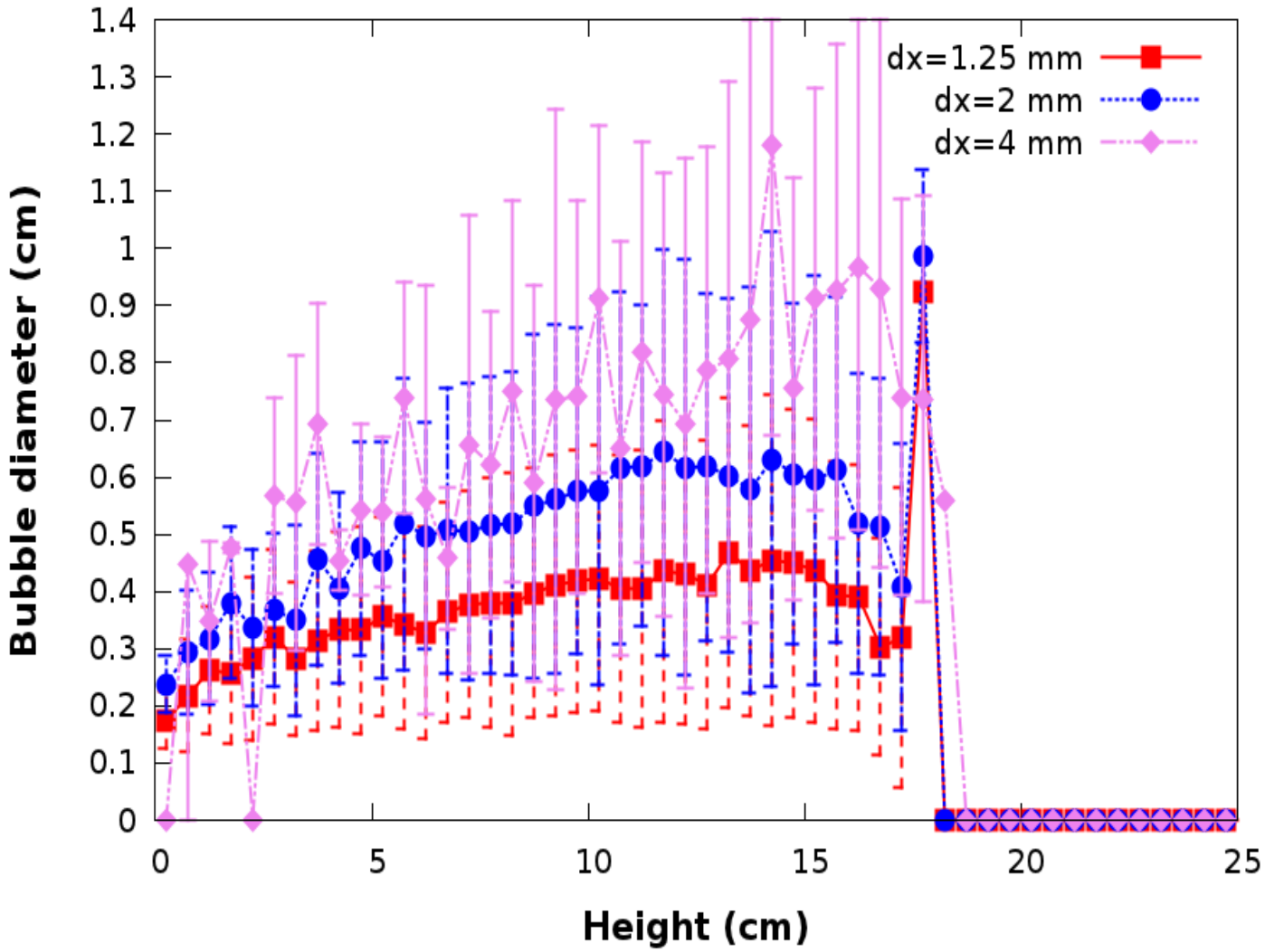
Condition\result	Exp. (PDT812)	Num.	Exp.(PDT850)	Num.
15 cm, 3 U_{mf}	139.3 ± 2.5	142	159.1 ± 2.3	180
15 cm, 5 U_{mf}	137.4 ± 4.1	146	168.5 ± 0.5	175
15 cm, 7 U_{mf}	138.5 ± 2.6	145	167.8 ± 0.5	175
20 cm, 3 U_{mf}	140.9 ± 3.2	145	249.4 ± 2.1	259
20 cm, 5 U_{mf}	141.3 ± 2.4	145	246.5 ± 1.6	268
20 cm, 7 U_{mf}	140.5 ± 1.9	146	249.2 ± 1.6	264



Voidage distribution and bubble predicted by different models

Grid Study Again





Snapshots of grid study (left) and bubble analyses (right)

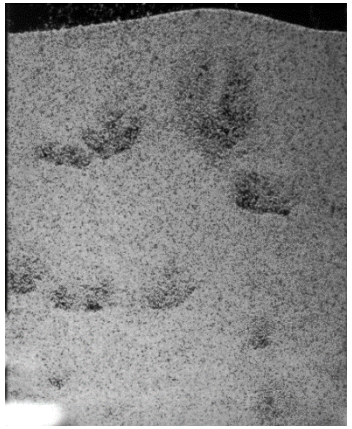
Takeaway

- **No good grid convergence for the current modeling of Group A particles**
  - Bed expansion tends to be over-predicted by TFM with homogeneous drag model
  - Bed heights keep decreasing with the grid refinement for both 2D and 3D simulations
  - Fine grid simulations predict small bubbles which were not likely observed in experiment
- **Coarse-grid simulations with heterogeneous drag, i.e. filtered drag, yield more realistic results**
  - Comparable bed expansion to experimental observation can be obtained
  - More realistic bubbling behavior in simulation can be obtained
  - Moderate grid dependence for bubble characteristics
- **Questions**
  - Are those small bubbles predicted by the fine grid simulations realistic?
  - If not, why would that happen?

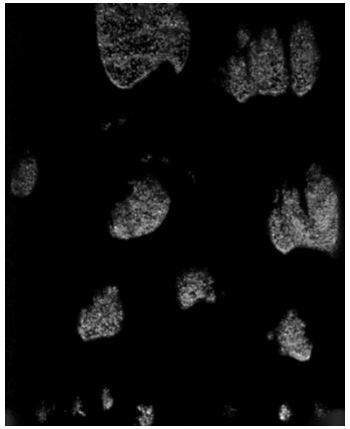
Pseudo-2D Column for Fine Particles

- **Pseudo-2D fluidized bed (Li et al. 2017)**
  - Dimension: 45 x 5 x 0.32 cm
  - Sieved FCC particles: 148 µm, 1300 kg/m^3, (U_{mf}=1.73 cm/s)
  - NETL 32D sorbents: 100 µm, 480 kg/m^3, (U_{mf}=0.23 cm/s)
- **Tests and measurements**
  - Various bed heights and gas velocities

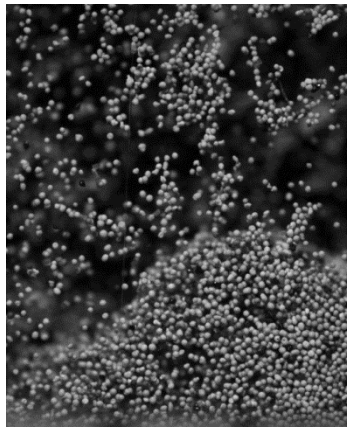
Flashing front light

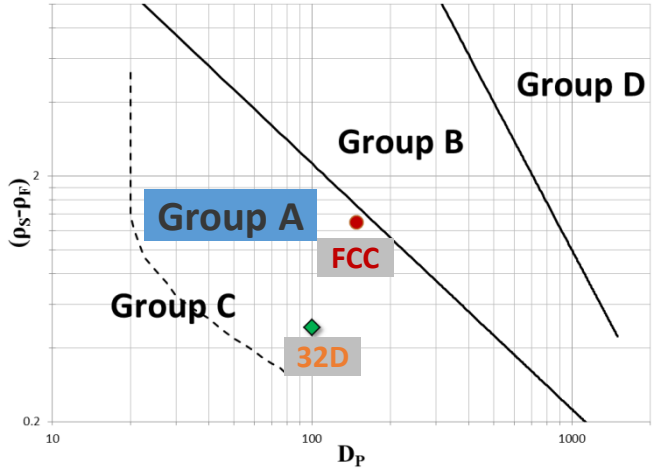


Flashing back light



Close view

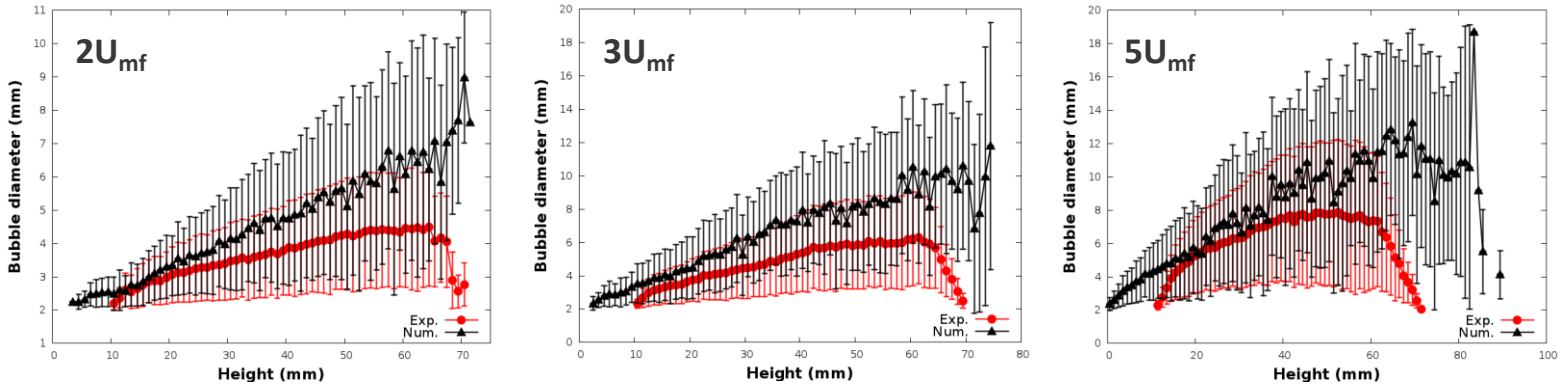




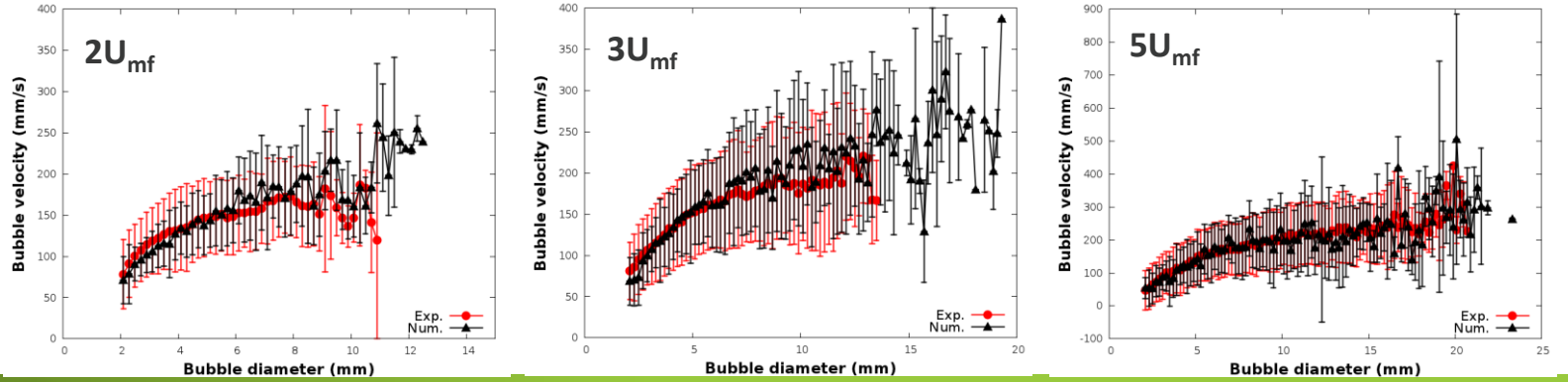
MFIX-DEM Simulations

- Non-cohesive FCC
  - U_g=2, 3, 5 U_{mf}
  - H=6 cm, 3.2M

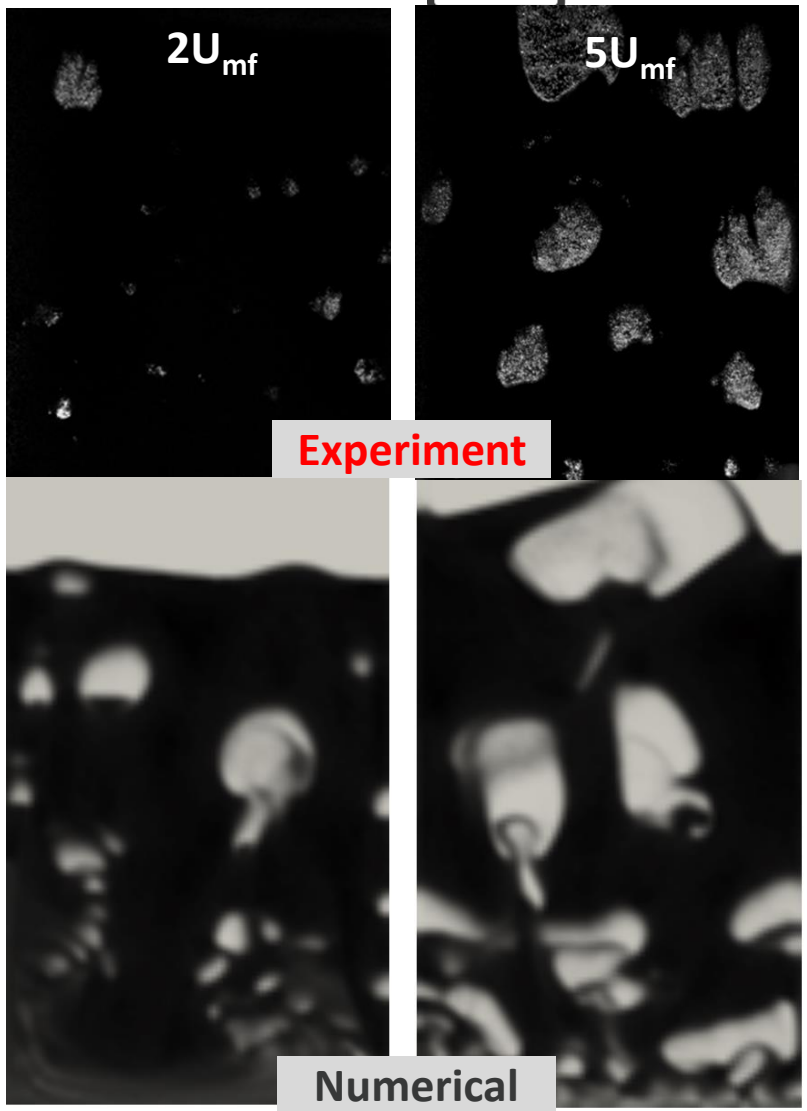
Gas Velocity	Exp. Bed Height (cm)	Num. Bed Height (cm)
2 U_{mf}	6.7	6.9
3 U_{mf}	7~7.3	7.2
5 U_{mf}	7.9~8.2	7.9



Bubble diameter along height

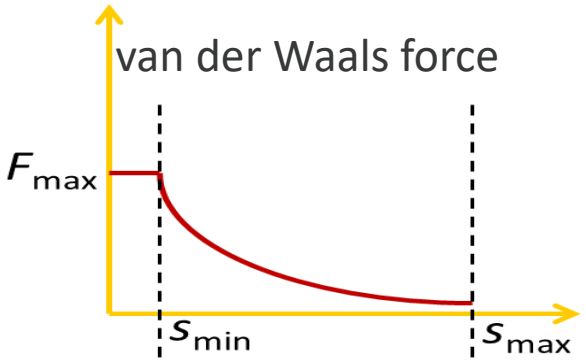


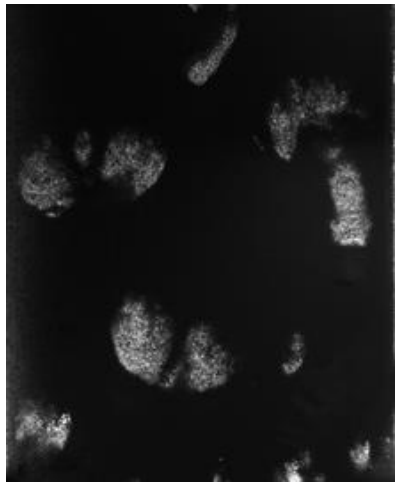
Bubble velocity versus bubble diameter



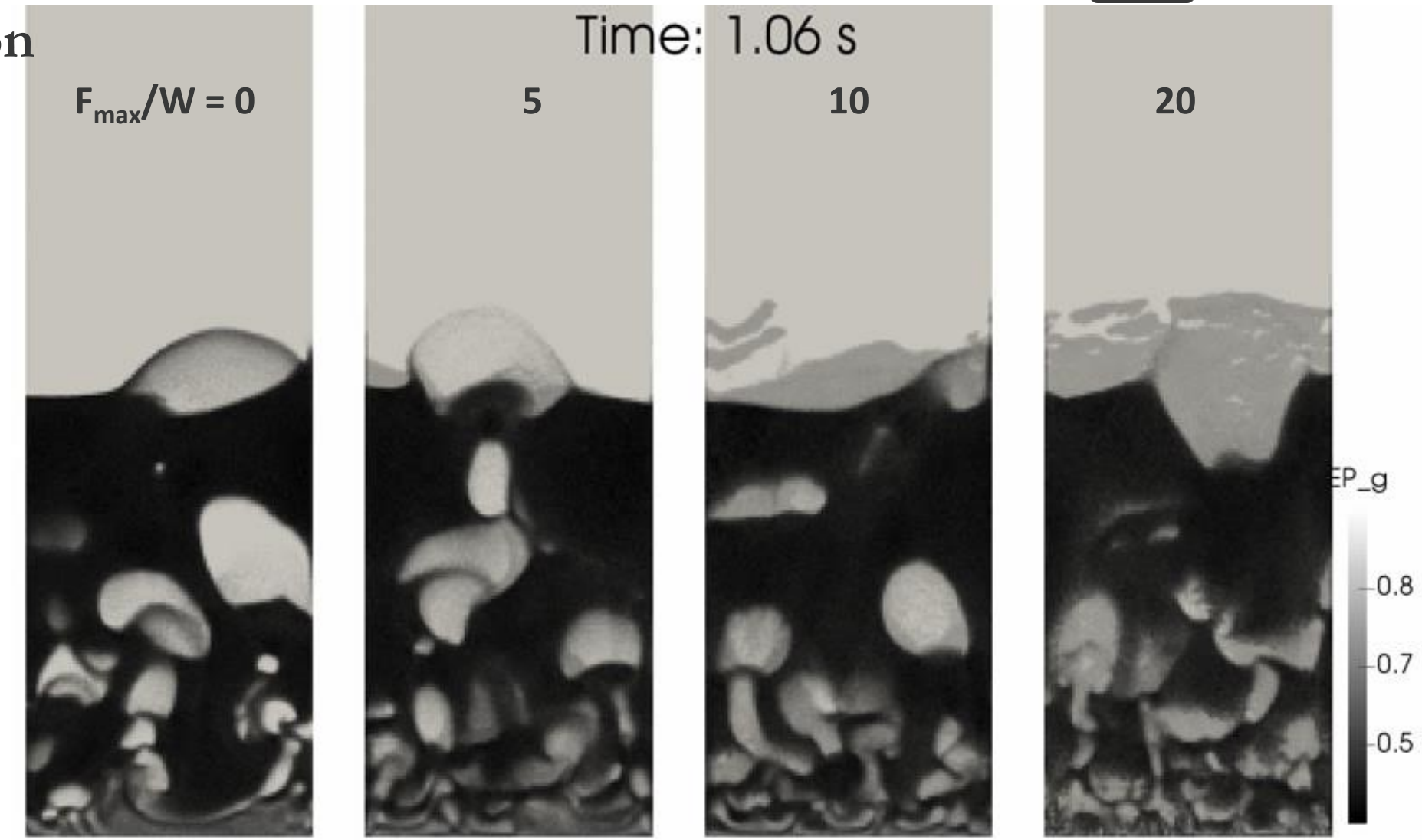
FCC Particles

- Effect of cohesion





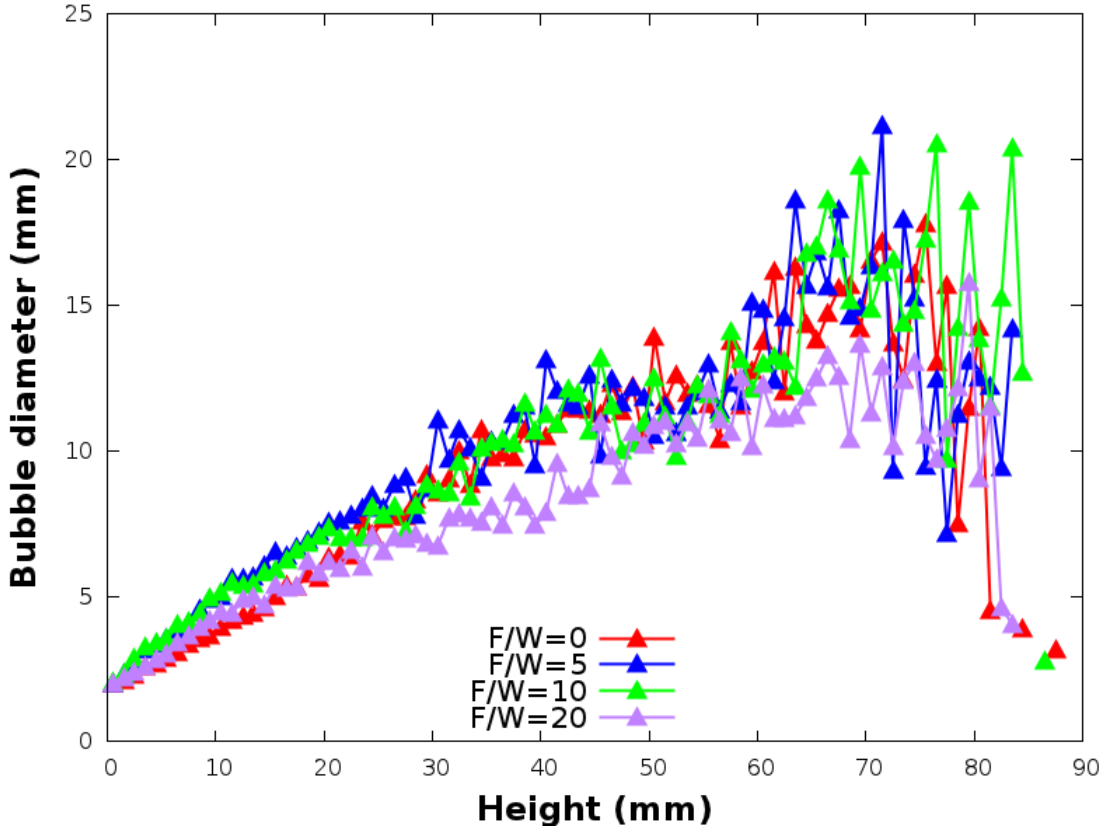
Experiment

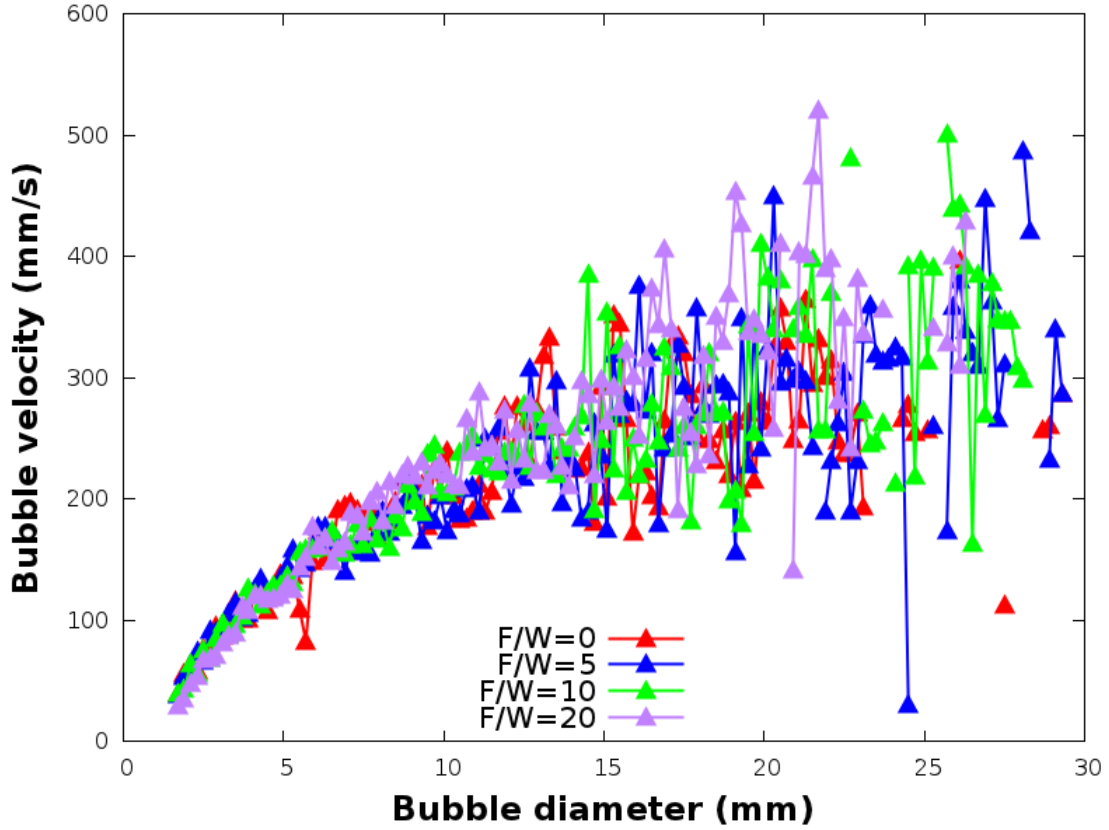


FCC Particles

- Effect of cohesion
  - Bubble analysis and bed height

Condition	Experiment (cm)	Prediction $F_{vdw,max}/W_p = 0$	Prediction $F_{vdw,max}/W_p = 5$
2 Umf	6.7	6.9	7.1
3 Umf	7–7.3	7.2	–
5 Umf	7.9–8.2	7.9	8.2

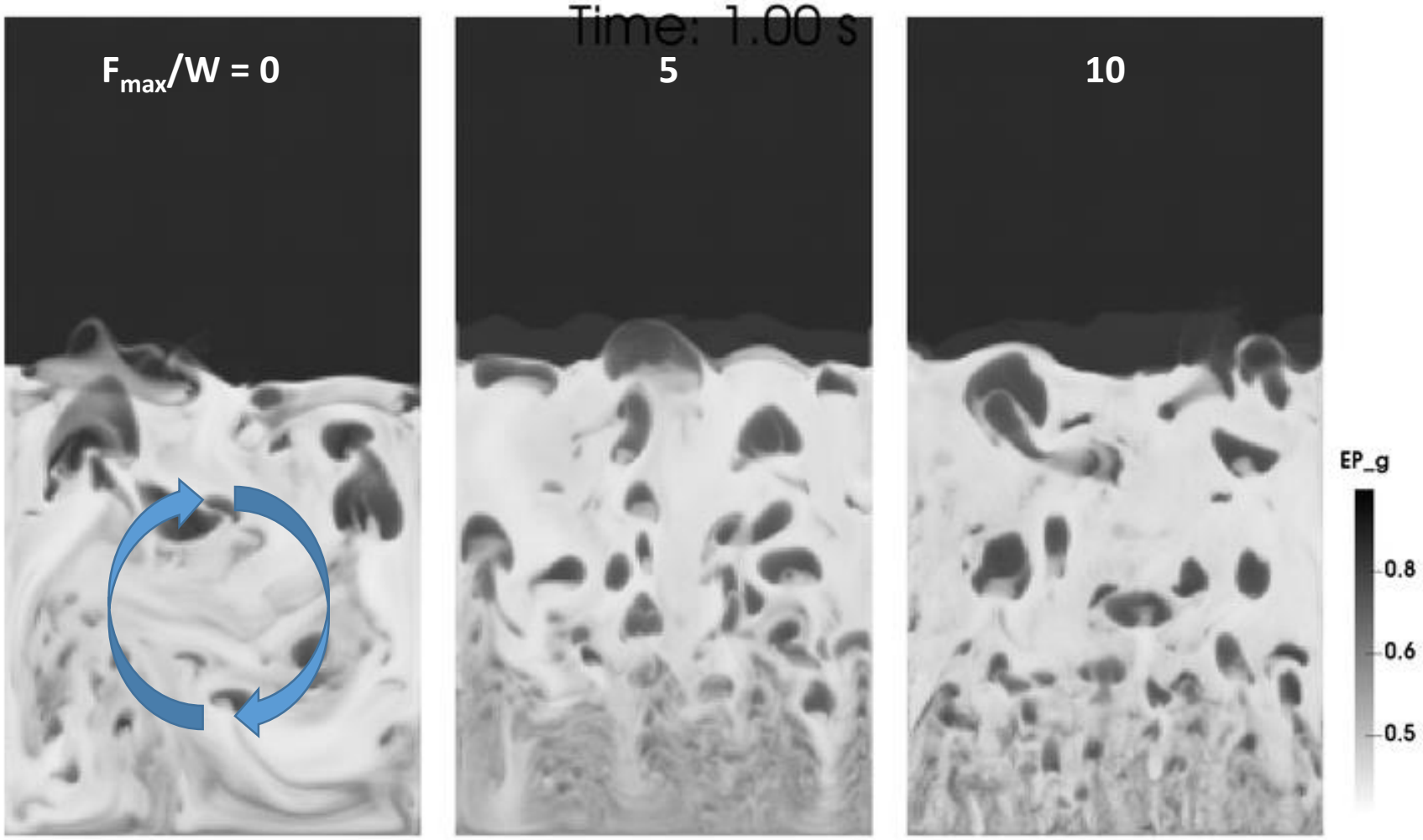




32D Sorbents

- 32D sorbents
  - U_g=11 U_{mf}
  - H=3.8cm, 7.2M

Experiment
H(cm): **~5.4**



5.5 **5.8** **5.8**

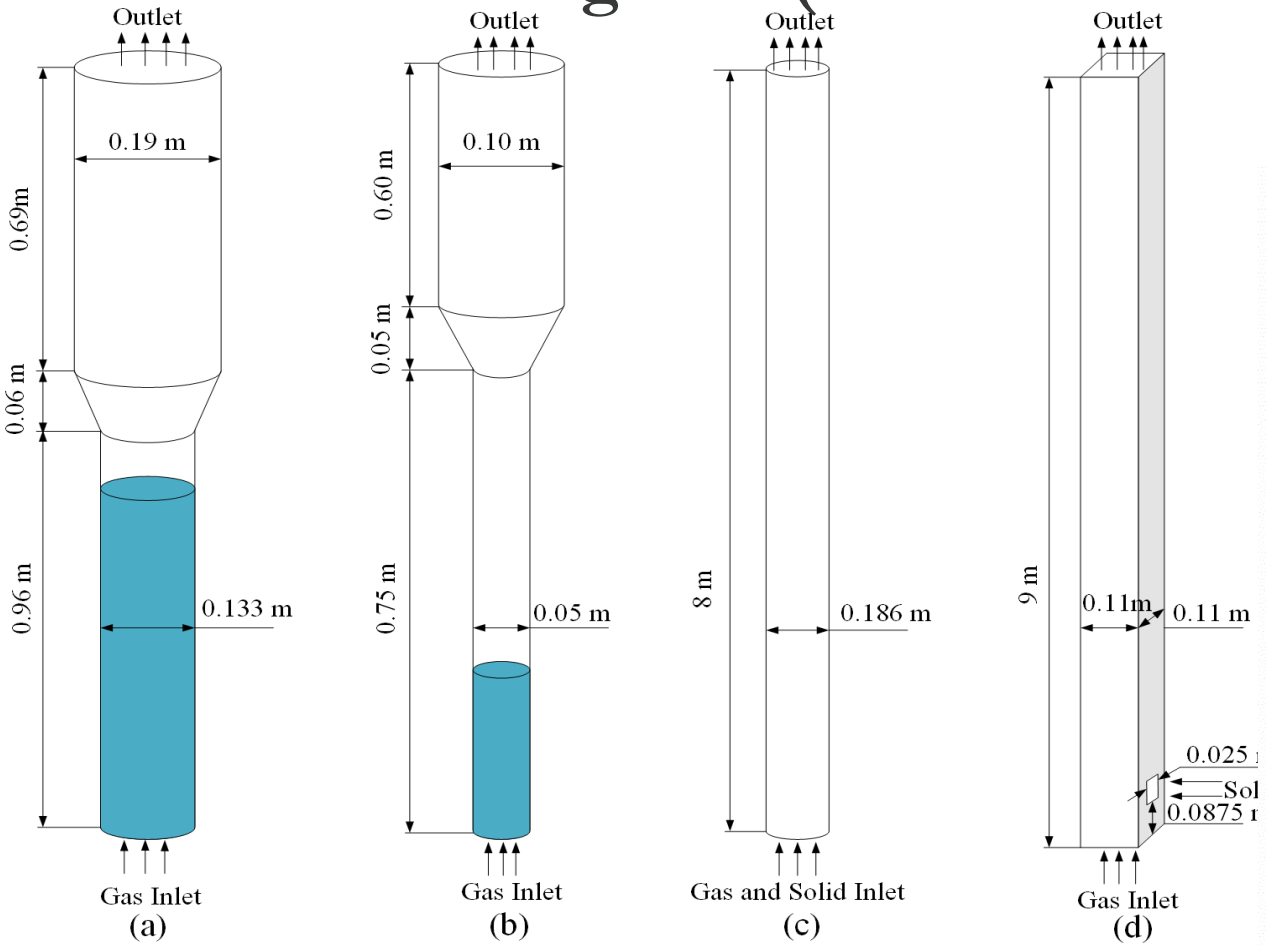
Volume rendering (X-ray image)

Takeaway

- **Bed expansions were reasonably predicted by MFIX-DEM simulations using homogeneous drag**
  - With and without inter-particle cohesive force
- **Bubble properties predicted are comparable with the experimental observation**
  - No small bubbles observed for 32D sorbents and FCC particles
- **Cohesive force has strong effects on bubbling pattern and solid internal circulation**
  - Stronger effect for fine 32D sorbents than for coarse FCC particles
- **Question**
  - How about PSD, particle shape, electro-static force, etc.?

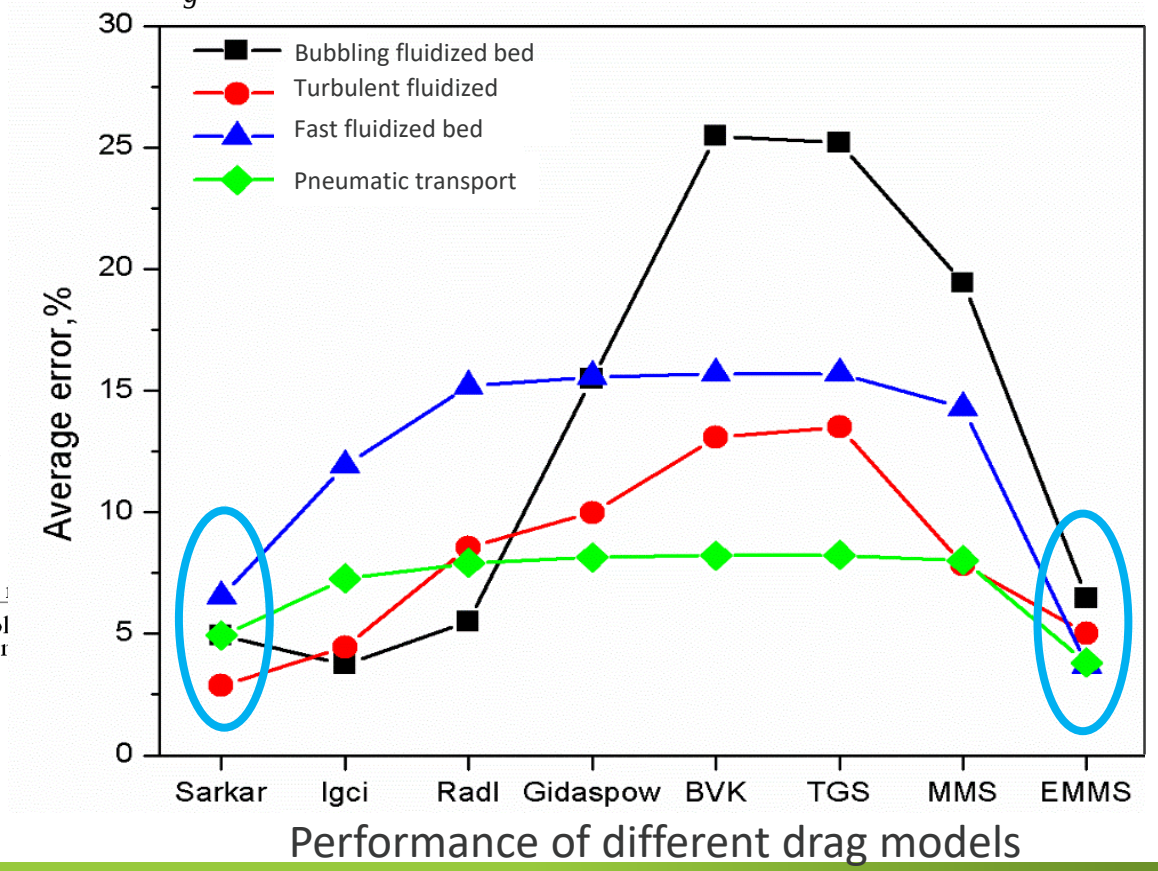
Drag Evaluation for Group A Particles

- Different flow regimes (Gao et al. 2018)



$$E_{abs} = \sum_{i=1}^{N} \frac{\left|\alpha^{i}_{g,sim} - \alpha^{i}_{g,\exp}\right|}{\alpha^{i}_{g,\exp} N}$$

α_g: axial gas holdup



Performance of different drag models

Concluding Remarks

- Many challenges in modeling Group A particles with different approaches
- Certain success can be achieved using the available modeling tools
- Heterogeneous drag is key to model fluidized bed applications when the fine-grid simulation is infeasible
- More detailed and reliable experimental data are always needed for model development and validation

Acknowledgement

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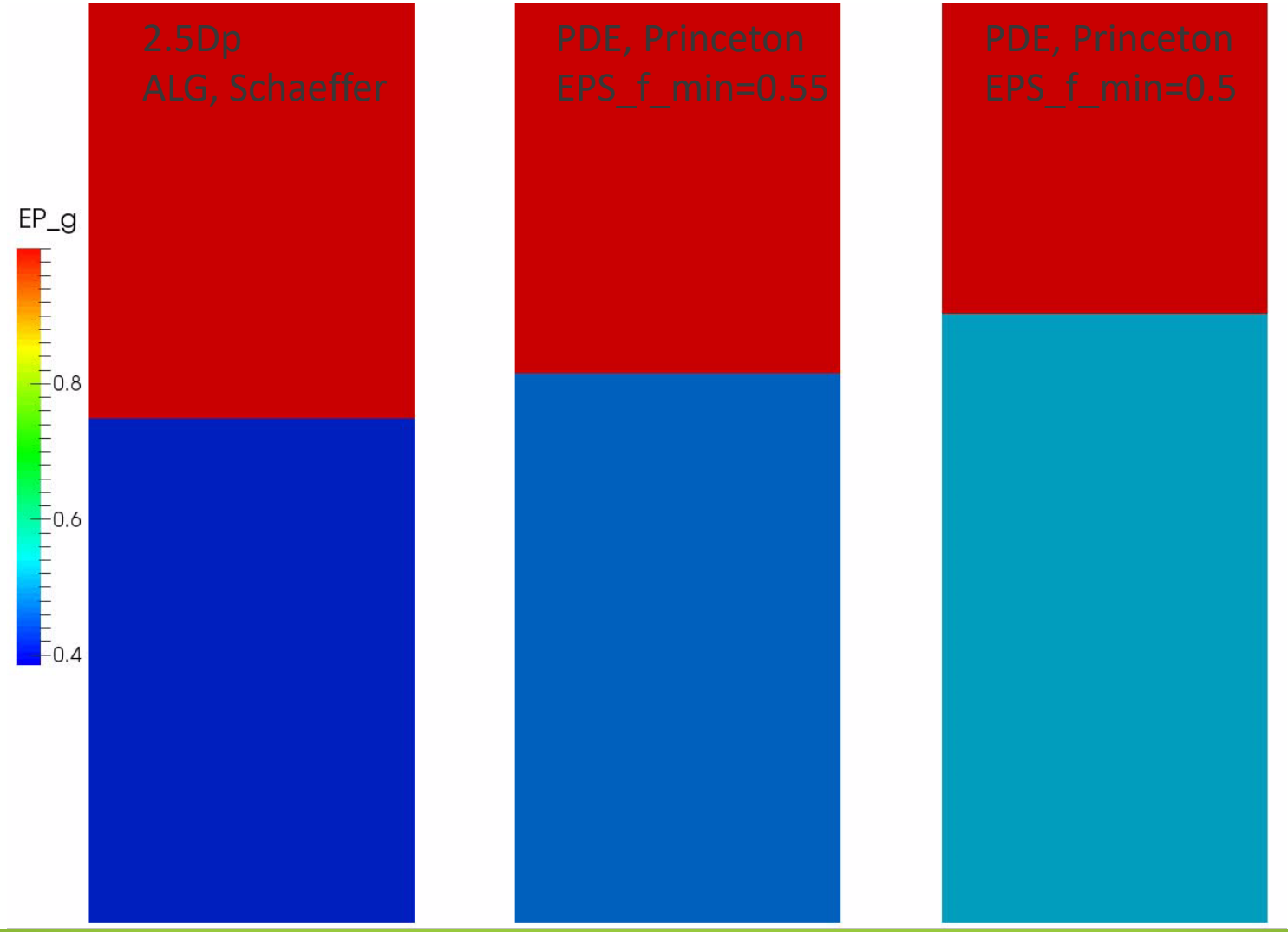
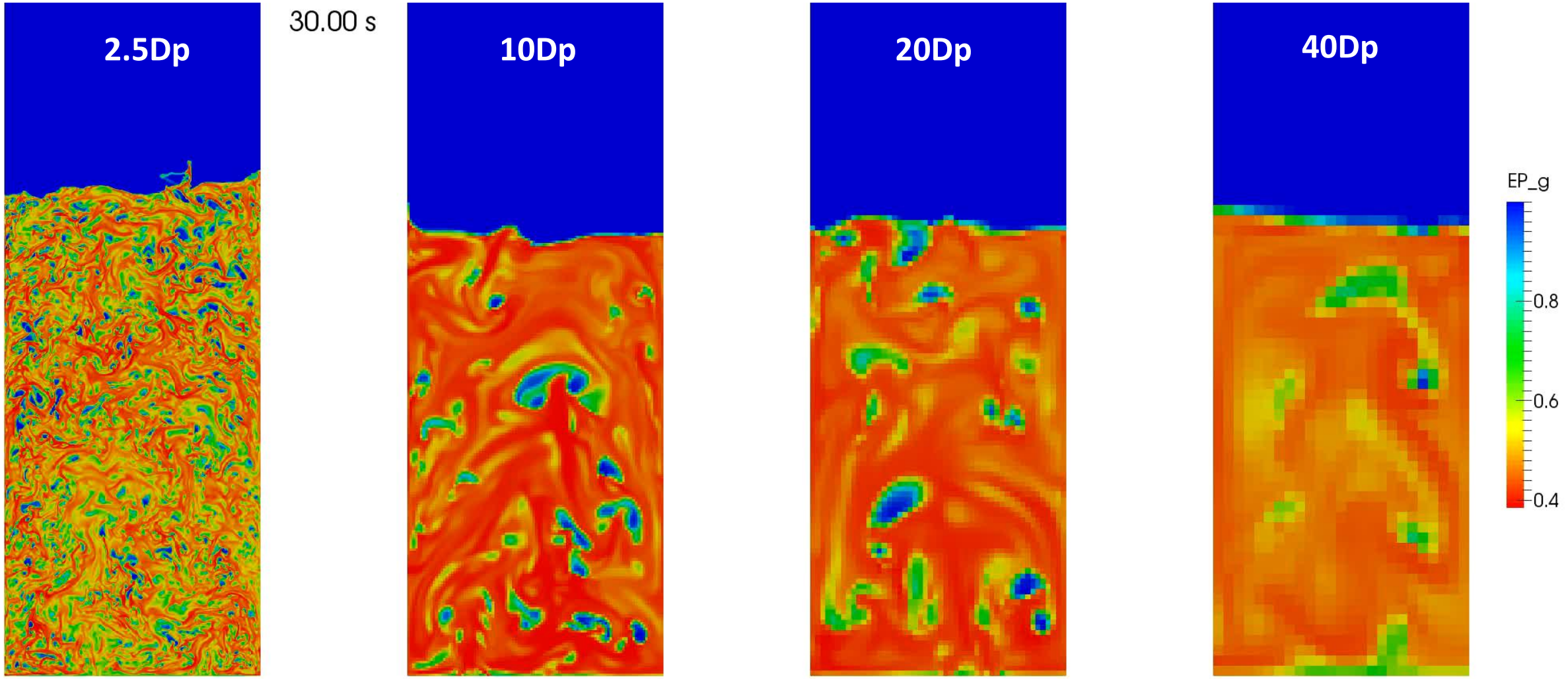
Backup Slides

Effect of Friction Model



2D Grid Study for Filtered Model



Further Grid Study

- **Simulation setup**
  - Domain: 2 x 10 cm
  - Same bed material and gas flow
  - Time-average voidage distribution
  - Verify when the bed height converges
- **Observation**
  - Bed height keep decreasing with grid refinement
  - No true convergence has been observed so far
  - Many extremely small bubbles (not shown here)