Estimating the Specularity Coefficient for the Accurate Simulation of Fluidized Beds of Different Surface-to-Volume Ratios

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NETL Workshop on Multiphase Flow Science
August 5-6 2014

The authors gratefully acknowledge **BP** for funding this research

Present Study

Objectives

i. To develop suitable metrics for quantifying the mixing of the solid phase
ii. To investigate the impact of wall boundary condition (specularity coefficient) on the hydrodynamics for fluidized beds of different surface-to-volume ratios

Overall

i. Circulation flux and bubble statistics tools to quantify hydrodynamics and mixing
ii. Wall boundary condition has significant impact on thin rectangular bed and cylindrical beds (diameters 14.5 and 30 cm)

The Two-Fluid Model

- Solid and gas phases fully interpenetrating continua using generalized NS equations
- Computationally efficient
- Conservation equations coupled with constitutive relationships

$$\frac{\partial}{\partial t}(\varepsilon_{sm}\rho_{sm}\vec{v}_{sm}) + \nabla\cdot(\varepsilon_{sm}\rho_{sm}\vec{v}_{sm}\vec{v}_{sm}) = \nabla\cdot\bar{\bar{S}}_{sm} + \varepsilon_{sm}\rho_{sm}\vec{g} + \vec{I}_{gm}$$

Solid Phase Stress Tensor

Particle-Particle Interactions

Drag Law

Particle-Gas Interactions

Plastic Flow

Viscous Flow

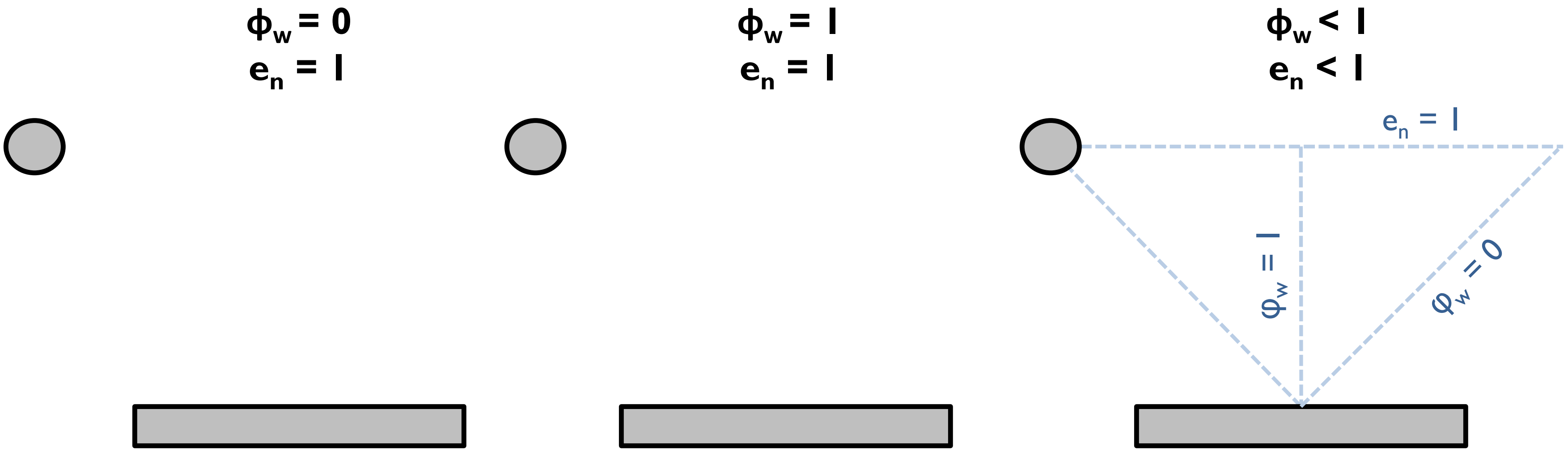
The TFM has been implemented using **MFiX** *(Multiphase Flow with Interphase eXchanges)*

Boundary Condition

Specularity Coefficient

- **Particle slip velocity** at wall using Johnson-Jackson[1] $\mathbf{n}\mu_s\nabla\mathbf{u}_s = -\frac{\pi\phi_w\mathbf{u}_s g_0\sqrt{3\Theta_w}}{6\epsilon_{s,max}}$
- ϕ = fraction of particle **tangential momentum** transferred to wall through collisions
- Friction neglected for simplification ⇒ ϕ includes frictional effects
- Indicative of **wall roughness**; also affected by superficial velocity, particle size
- $\phi_w \in [0,1]$ such that $\phi_w = 0$ ⇒ Free slip along the wall, minimum hindrance

  $\phi_w = 1$ ⇒ Zero tangential velocity, maximum hindrance

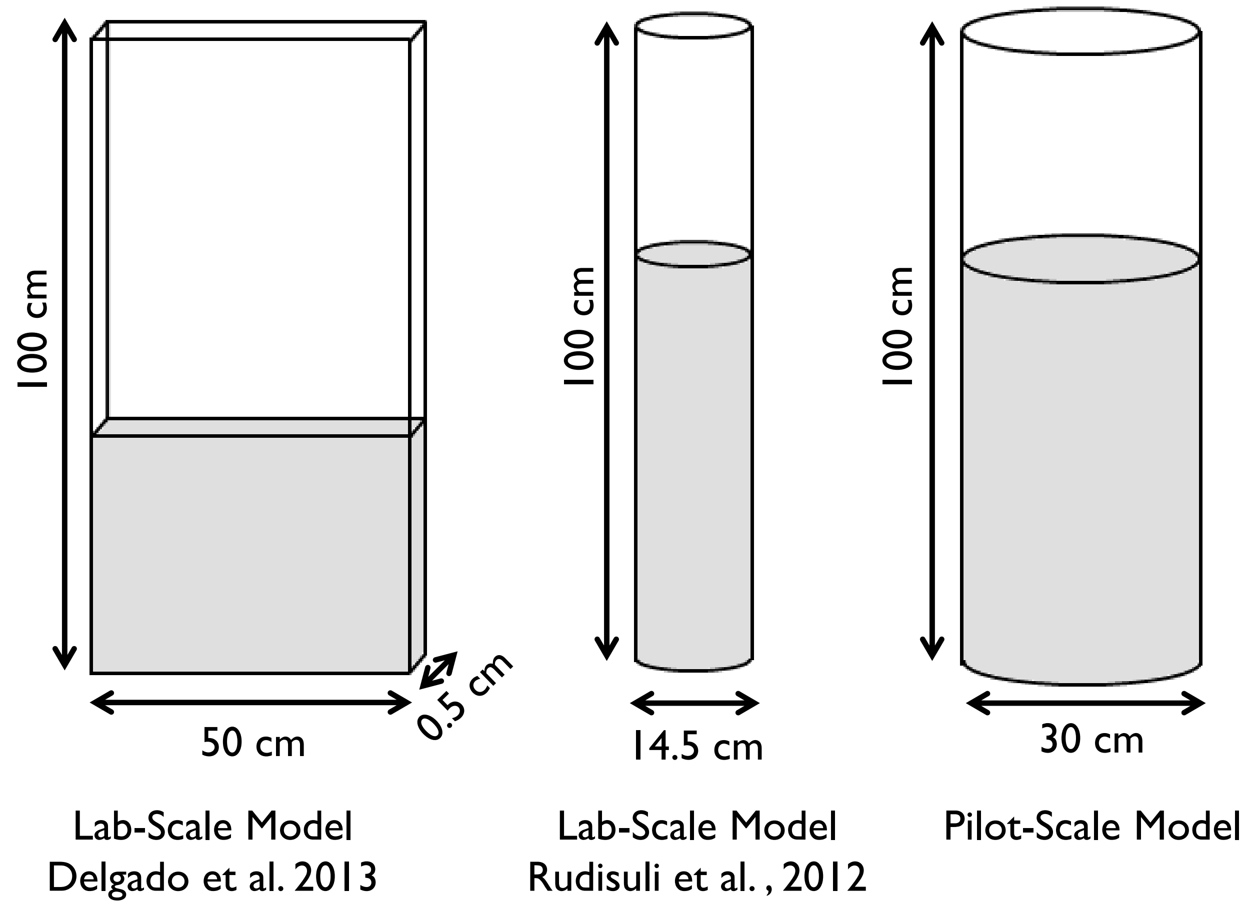


Parametric Analysis

- Lack of experimental data on ϕ_w => ϕ_w is a fitting parameter

ϕ_w *tuned to* 2D simulations is not appropriate for 3D simulations

- Thin rectangular beds extensively used in **experimental studies** employing non-intrusive measurements techniques
- Cylindrical beds **more realistic** geometries for scale-up and different hydrodynamics compared to pseudo-2D beds
- Variation of specularity coefficient to evaluate impact on simulation of pilot-scale model

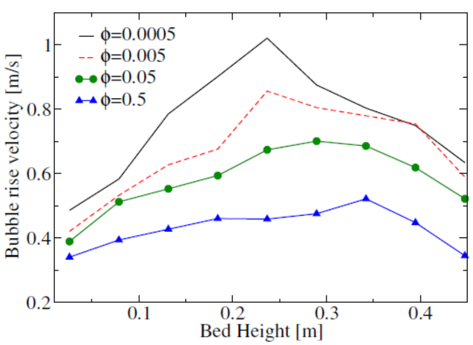


Metrics for Fluidization

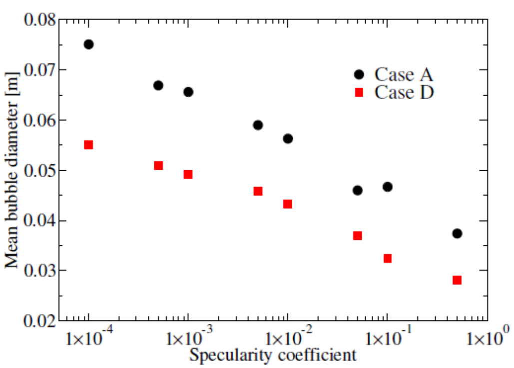
Original CFD data *f(x,y,z,t)*

Bubble statistics

Velocimetry → **Velocity vs Height**

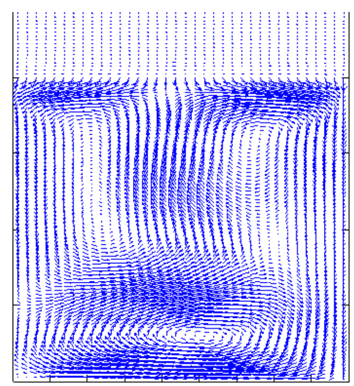


Static → **Size vs height**

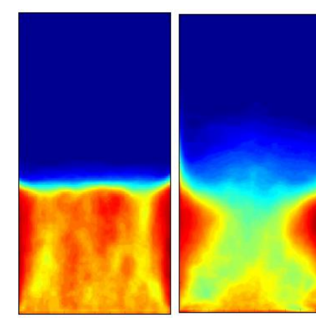


Dense phase statistics

Velocimetry → **Circulation flux**



Static → **Time mean solids holdup**

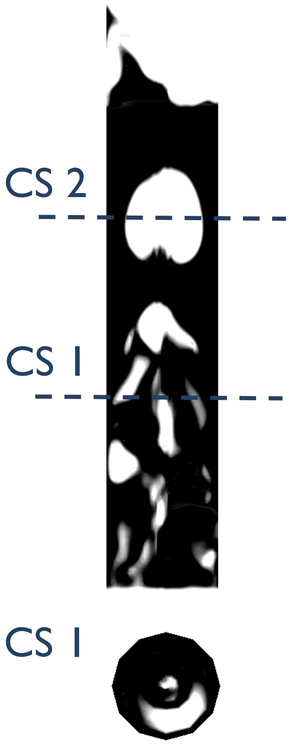


Metrics for Fluidization

Bubble Statistics

Simulation

2D Vertical Slice or Cross Section using simulation data



Digital Image Analysis

Bubble detection using ImageJ

Threshold void fraction = 0.7

Min bubble diameter = 1 cm

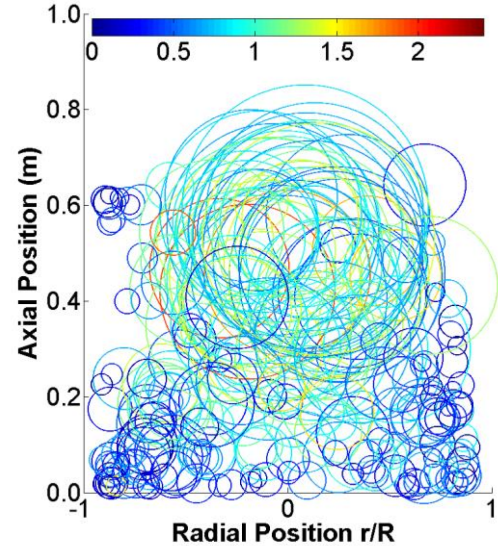
Bubble statistics using MATLAB

Lagrangian Velocimetry

Bubble numbering based on lateral and axial positions

Velocity using identical numbered bubbles in consecutive frames

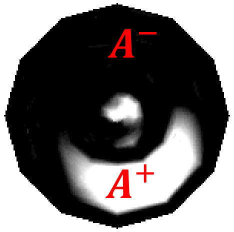
Filters to remove unphysical bubble velocities



Circulation Flux and Time

Time mean **solid's circulation flux up** $J_c^+(y)$ based on the upflow area $A^+(y)$ i.e.

$$J_c^+(y) = \left\langle \frac{1}{A^+(y,t)} \int\int \rho_s \cdot \varepsilon_s^+ \cdot V_s^+ \ dz^+ dx^+ \right\rangle$$



Define incremental positive circulation time such that

$$\Delta t_c^+(y) = \left\langle \frac{1}{A^+(y,t)} \int\int \frac{m^+(x,y,z,t)}{\dot{m}^+(x,y,z,t)} \ dz^+ dx^+ \right\rangle = \left\langle \frac{1}{A^+(y,t)} \int\int \frac{\Delta y \ dz^+ dx^+}{v_m\ (x,y,z,t)} \right\rangle$$

Positive circulation time t_c^+ is the average time taken by particles to reach axial height y_1 from the bottom of the bed i.e.

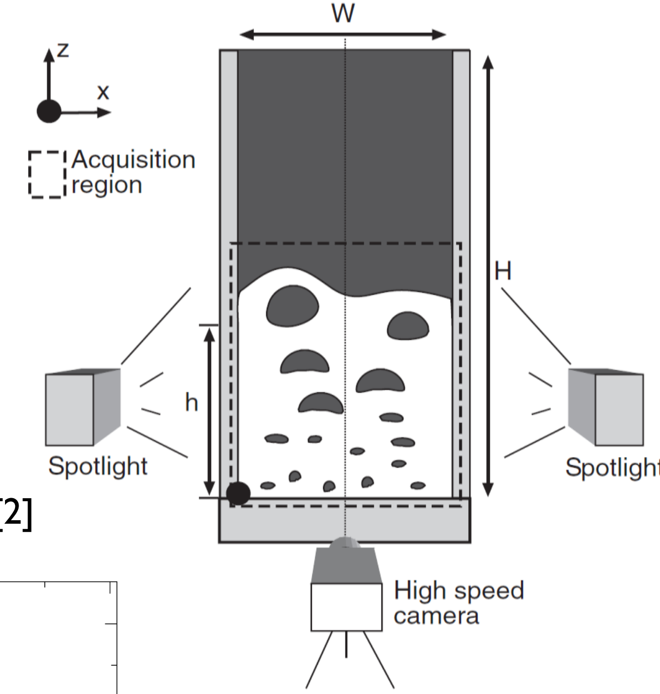
$$t_c^+|_{y_1} = \int_0^{y_1} \Delta t_c^+(y)\ dy$$

The total **solid's circulation time** $t_c|_{y_1} = t_c^+|_{y_1} + t_c^-|_{y_1}$ is representative of the mixing time scale

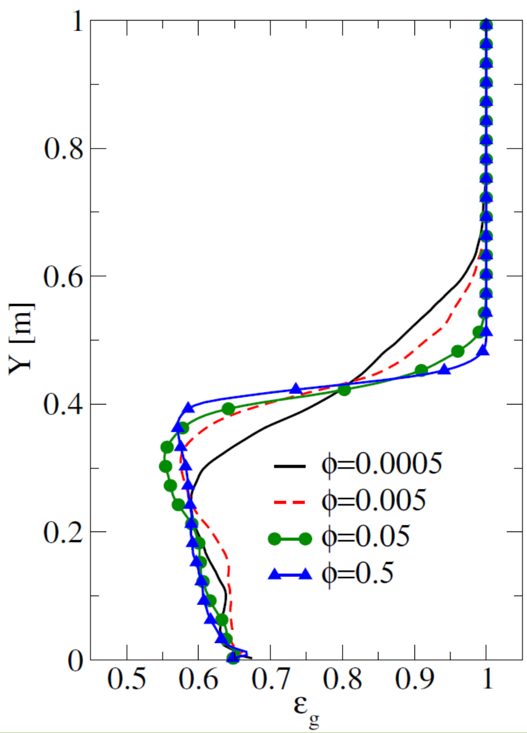
Thin Rectangular Bed

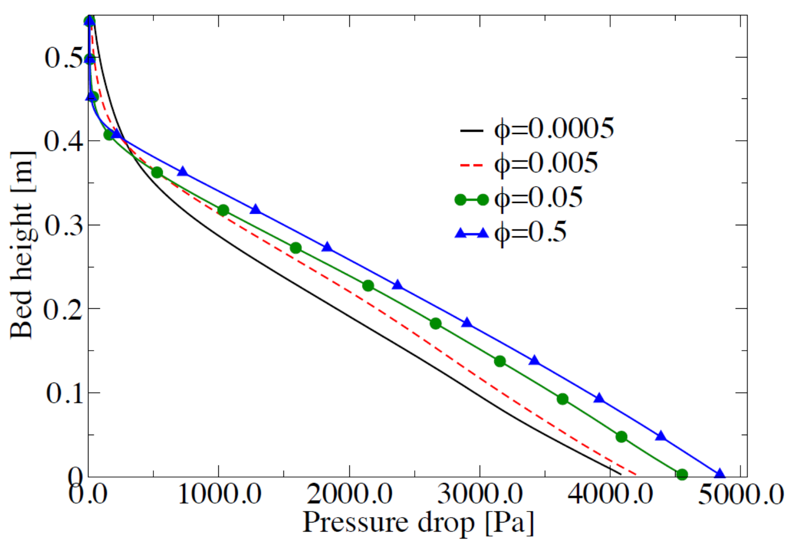
Experimental Conditions

Column	50 cm x 100 cm x 0.5 cm
Particles	Glass - d_p=678 μm, ρ_p=2500 kg/m^3
Static Bed Height	30 cm



Schematic of the experimental setup by Sanchez-Delgado et al 2013 [2]





Time mean void fraction and pressure drop profiles for U=2.5Umf

Simulation Results

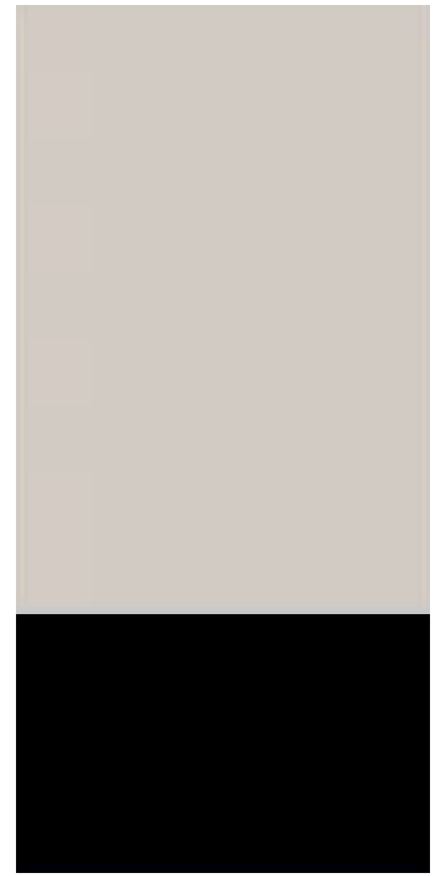
Bubble hydrodynamics and solids motion significantly influenced by wall boundary condition

$U_{in} = 2.5U_{mf}$
$\phi = 0.0005$

Negligible hindrance

$U_{in} = 2.5U_{mf}$
$\phi = 0.5$

Significant hindrance



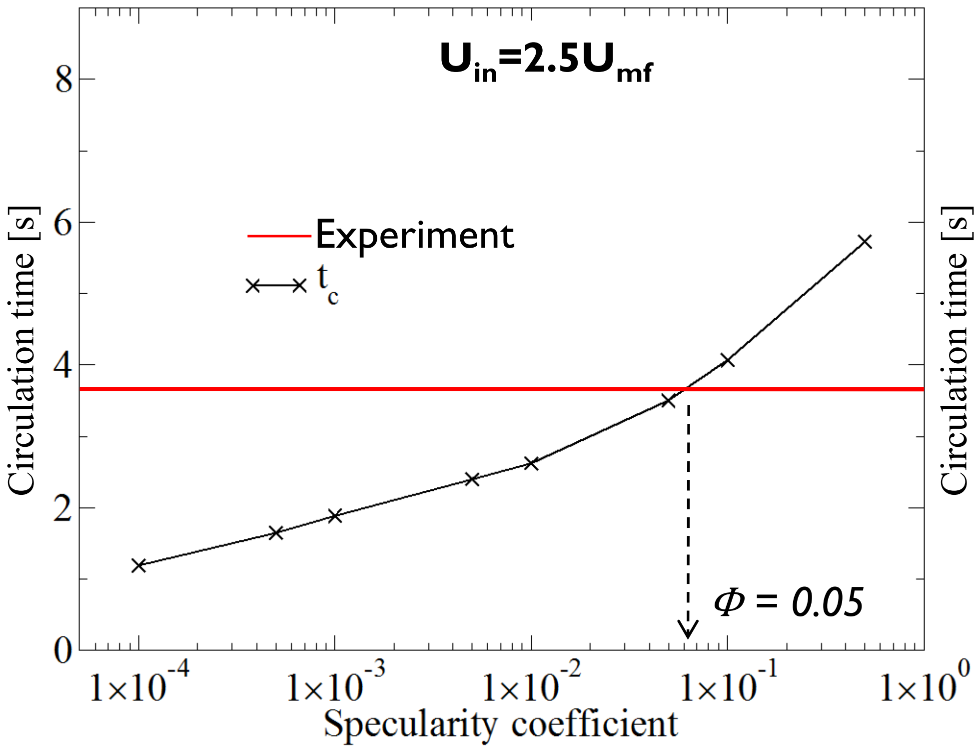
Decreasing ϕ results in:

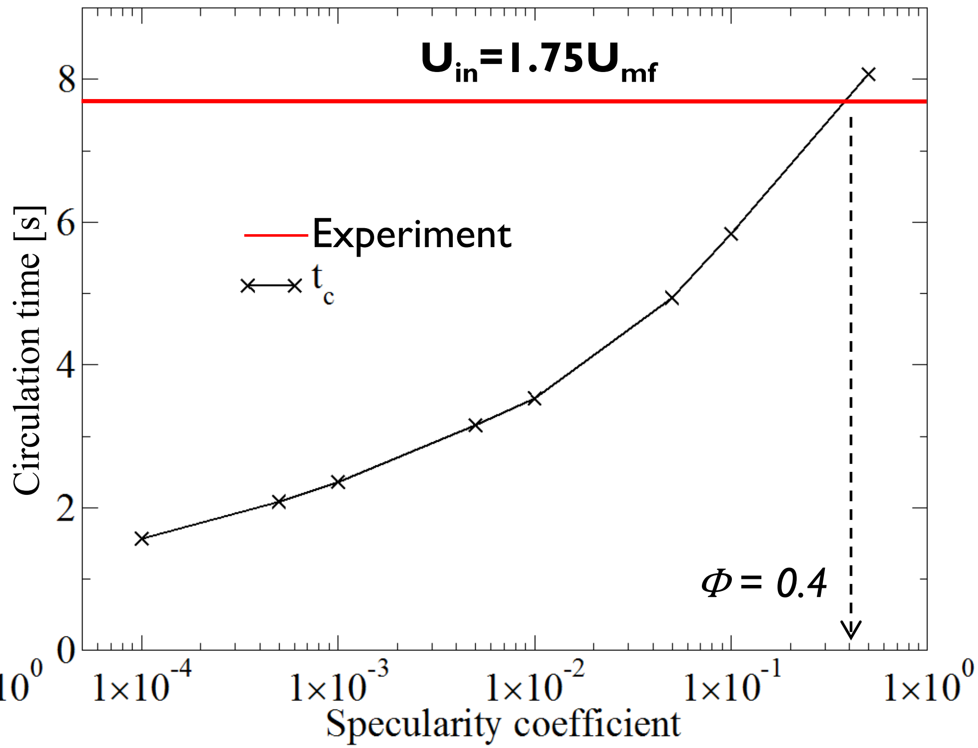
- Larger bubble sizes
- Slugging fluidization
- Gas bypassing effects
- Higher bubble velocities

Thin Rectangular Bed

Choosing Φ

- Circulation time ↑ when
  - U_{in} ↓ - closer to U_{mf} and less bubbling
  - ϕ ↑ - wall resistance increases ⇒ less solid motion close to walls and smaller bubbles
- **Appropriate ϕ ↓ as U_{in} ↑**. For the range, $1.5U_{mf} – 2.5U_{mf}$, Φ ∈ **[0.05,0.5]**





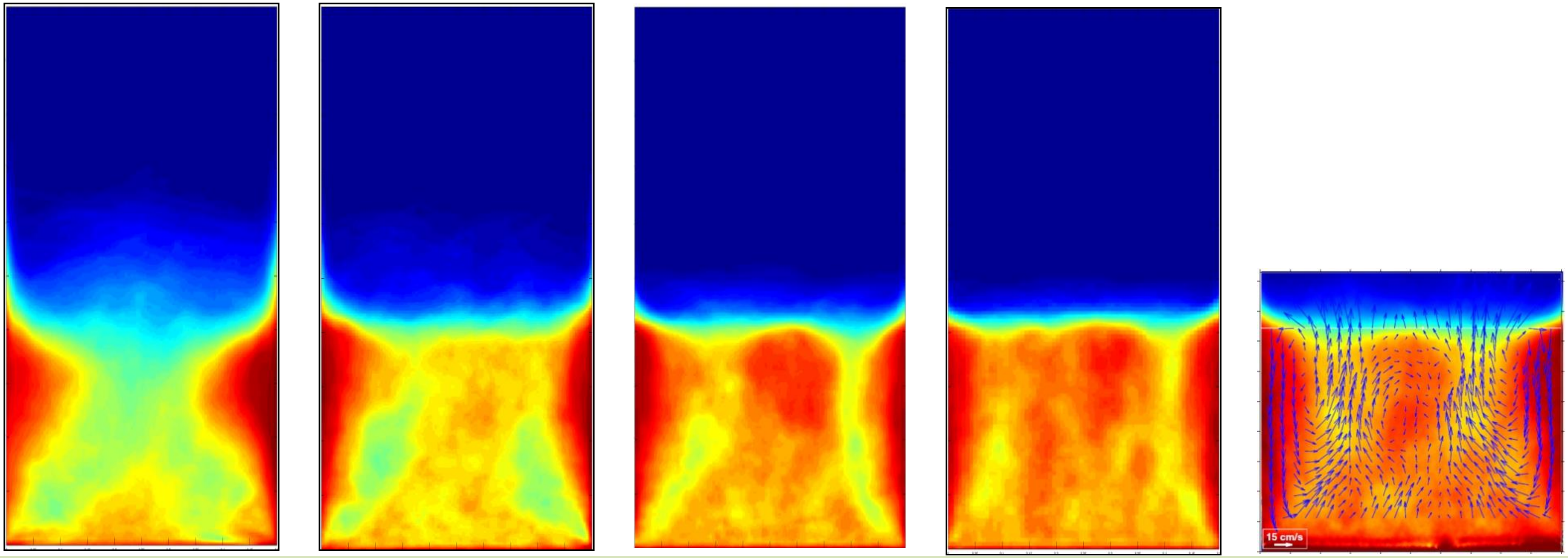
Thin Rectangular Bed

Solids Concentration Map

- Time average probability of solids phase based in the bed
- Distinct bubble pathways identified in all cases
- Cross validation study to verify appropriate specularity coefficient based on time mean metrics

Qualitative agreement for $U_{in} = 2.5U_{mf}$ using **Φ = 0.05**

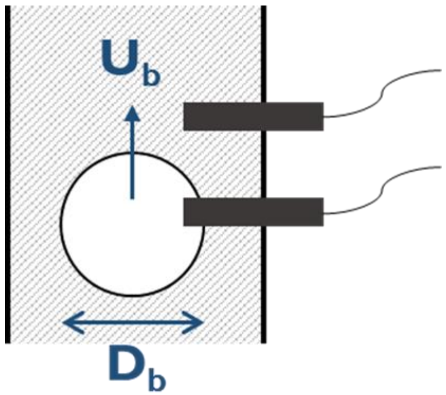
1E-3 **1E-2** **5E-2** **1E-1** **Experiment [2]**



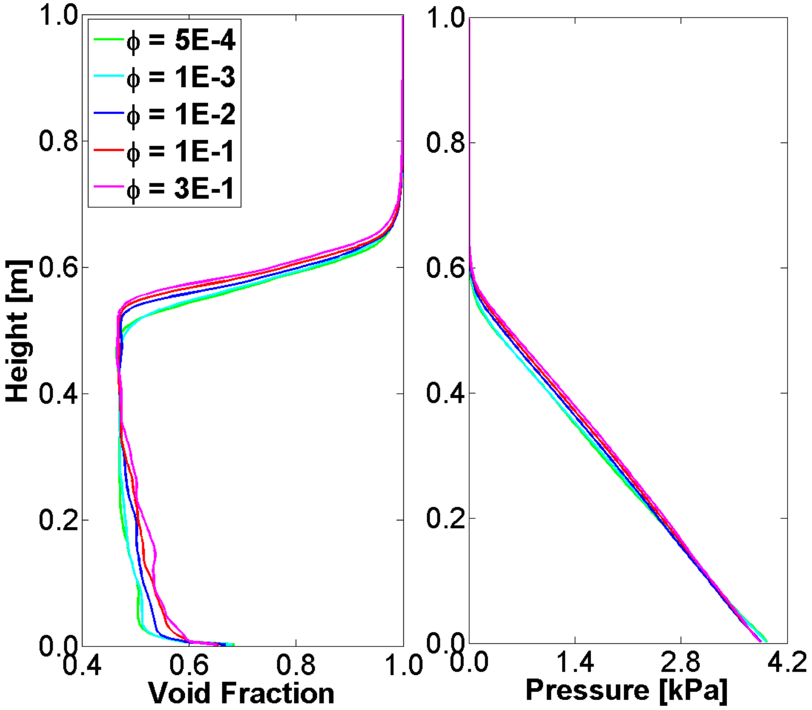
Lab-Scale Cylindrical Bed

Experimental Conditions

Column	D=14.5 cm, H=100 cm
Particles	Alumina - **d_p=289 μm, ρ_p=1350 kg/m^3**
Static Bed Height	50 cm
Measuring Level	23 cm, 45 cm



Optical probes used to study bubble growth and bubble velocity in the experimental setup by Rudisuli et al 2012 [3]



Time mean void fraction and pressure drop profiles for U=4.6Umf

Lab-Scale Cylindrical Bed

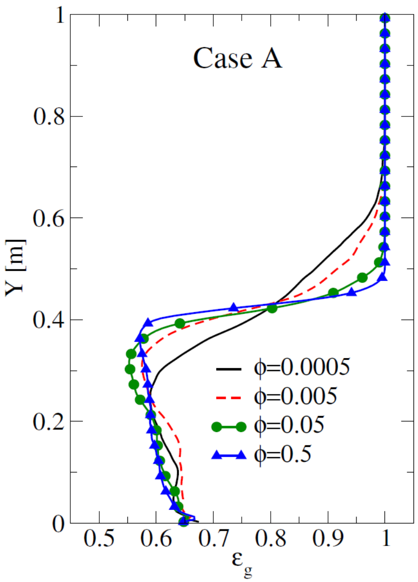
Experimental Conditions

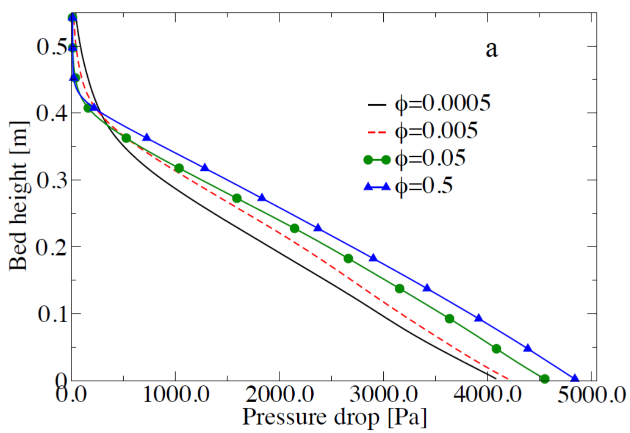
Column D=14.5 cm, H=100 cm

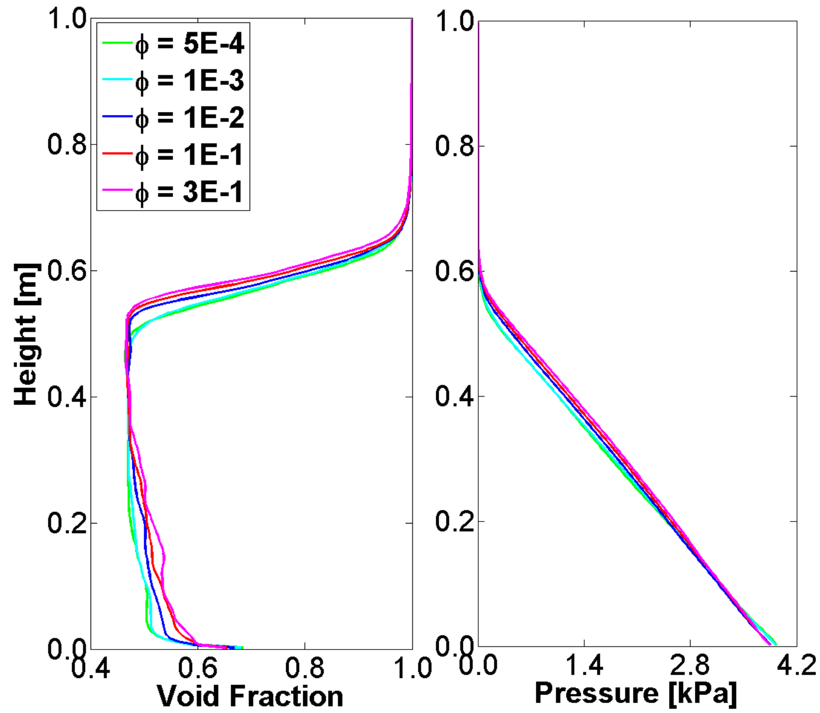
Particles Alumina - d_p=289 μm, ρ_p=1350 kg/m^3

0 cm

23 cm, 45 cm







Time mean void fraction and pressure drop profiles for U=4.6Umf

Lab-Scale Cylindrical Bed

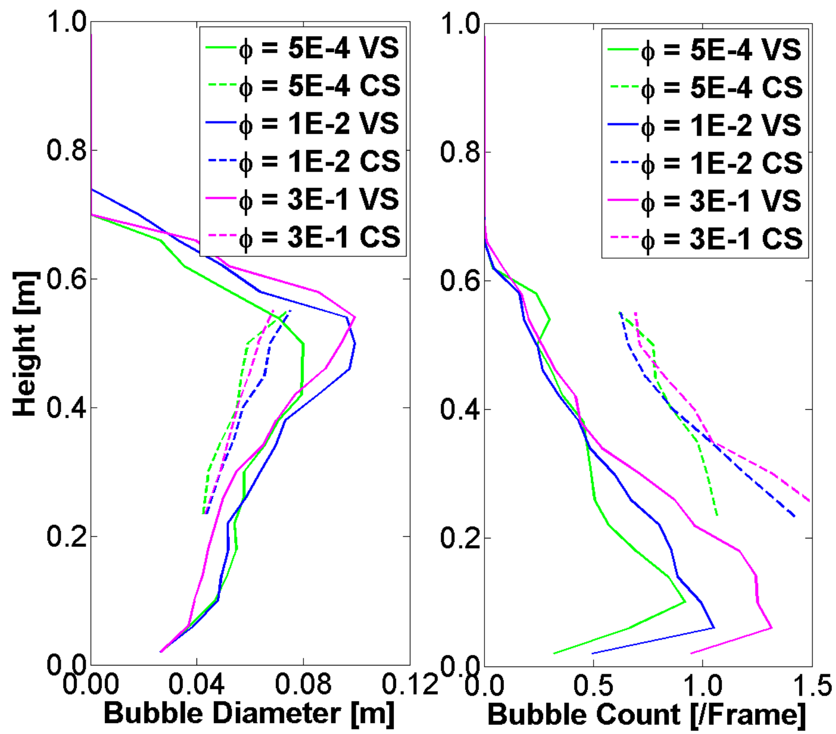
Simulation Results

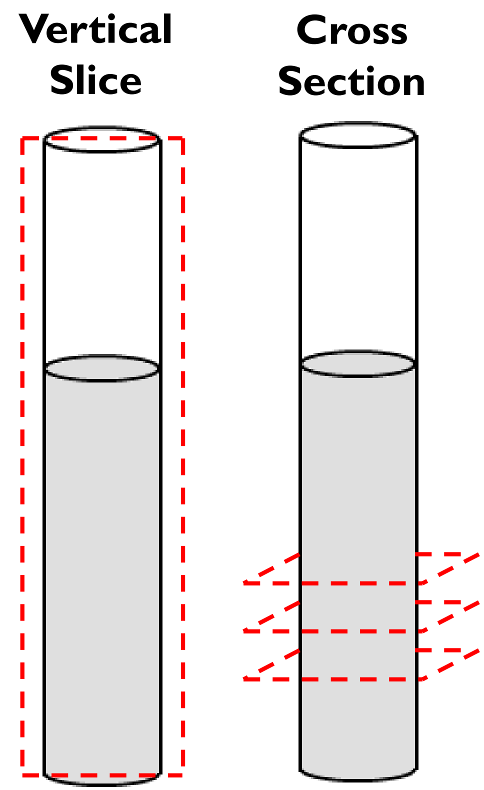
Data collected at 100 Hz for 3-30 s (**2700 frames**) for bubble statistics for 3.5, 4.6, 6.8 Umf

3D statistics on 2D planes ?

Bubble diameter plots predict same trends although VS yields cord length while CS yields bubble area

VS bubble count qualitatively matches CS bubble count (actual)

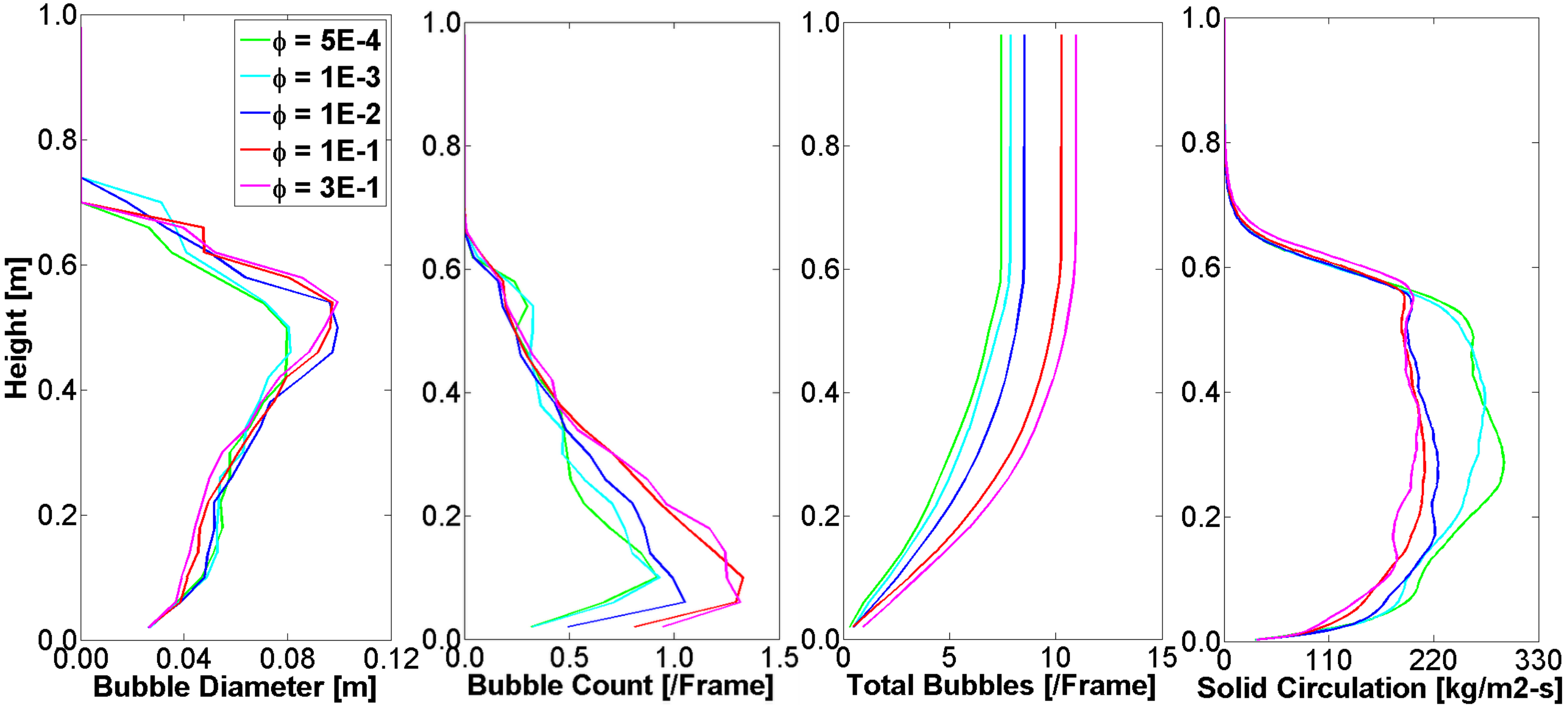




Lab-Scale Cylindrical Bed

Simulation Results

- Significant impact of specularity coefficient on bubble statistics and circulation fluxes
- **Unlike rectangular bed, higher Φ => more bubbles and bigger bubbles**
- Higher Φ => More resistance from walls => Lower solid circulation



Lab-Scale Cylindrical Bed

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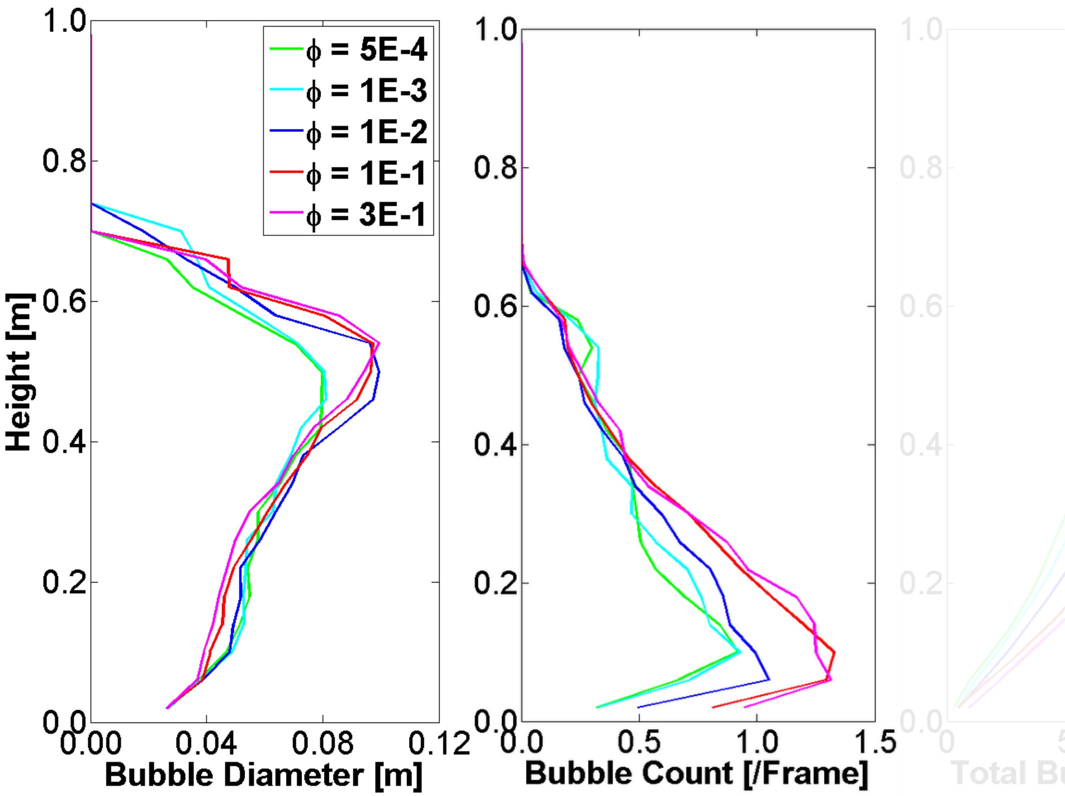
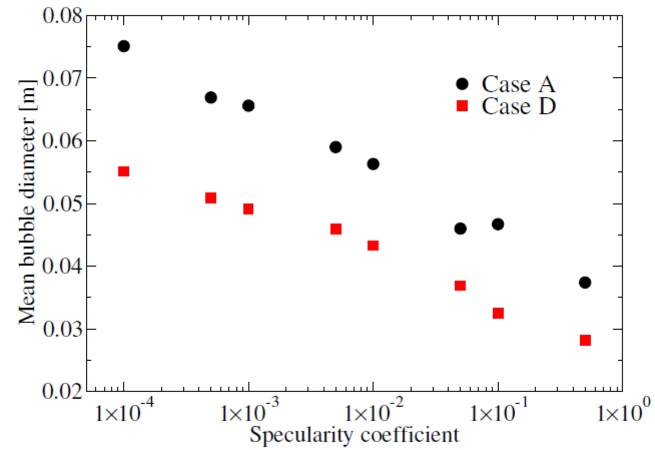
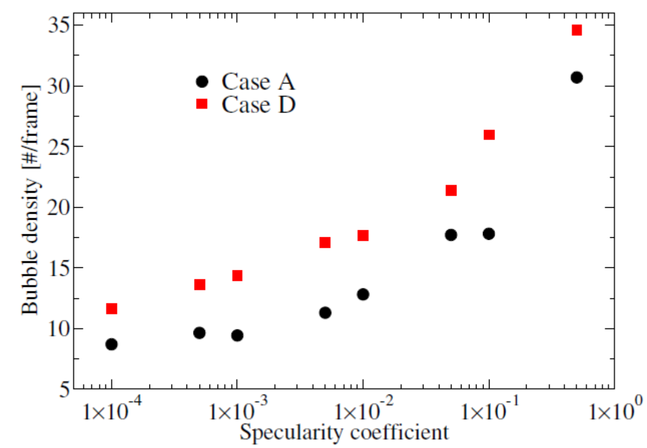






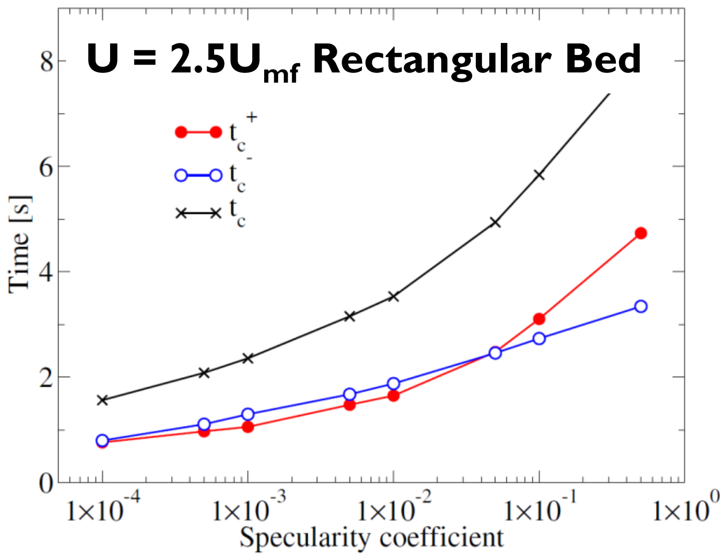
Lab-Scale Cylindrical Bed

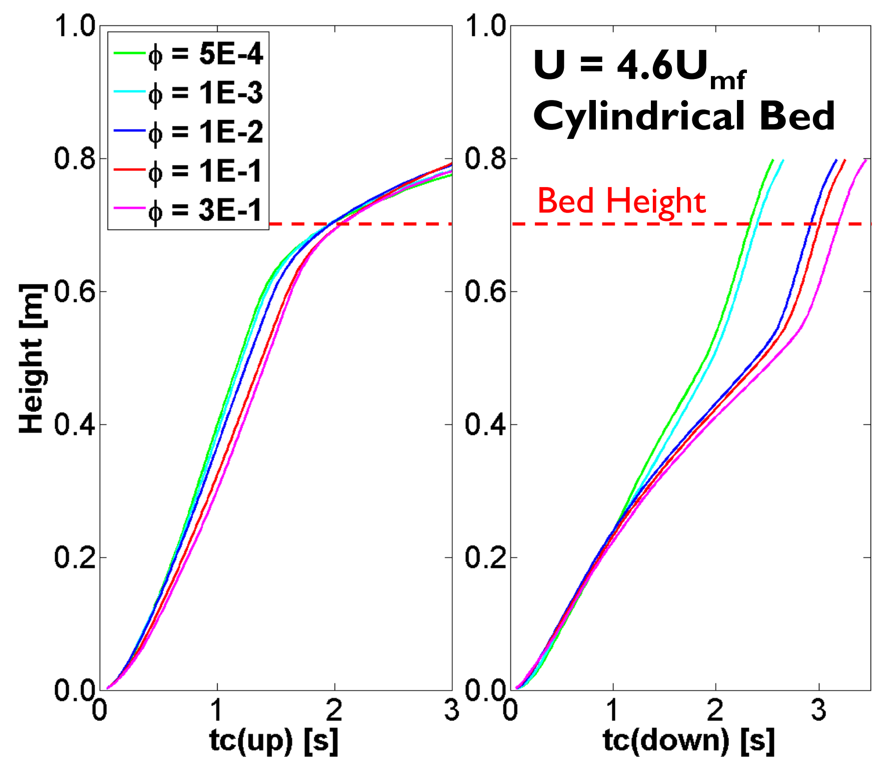
Circulation Time

- Important for predicting residence time of various components in different parts of the bed
- tc_{down} , tc_{up} and tc decrease with increasing U_{in}
- No effect of Φ on tc_{up} => bubbling behavior does not directly affect solid bulk motion !
- tc_{down} is more sensitive to Φ since solid particles fall along the walls
- Similar trends for 3.5 U_{mf} , 6.8U_{mf}

$$\Delta t_c^+(y) = \left\langle \frac{1}{A^+(y,t)} \int\int \frac{\Delta y \ dz^+ dx^+}{v_m\,(x,y,z,t)} \right\rangle$$

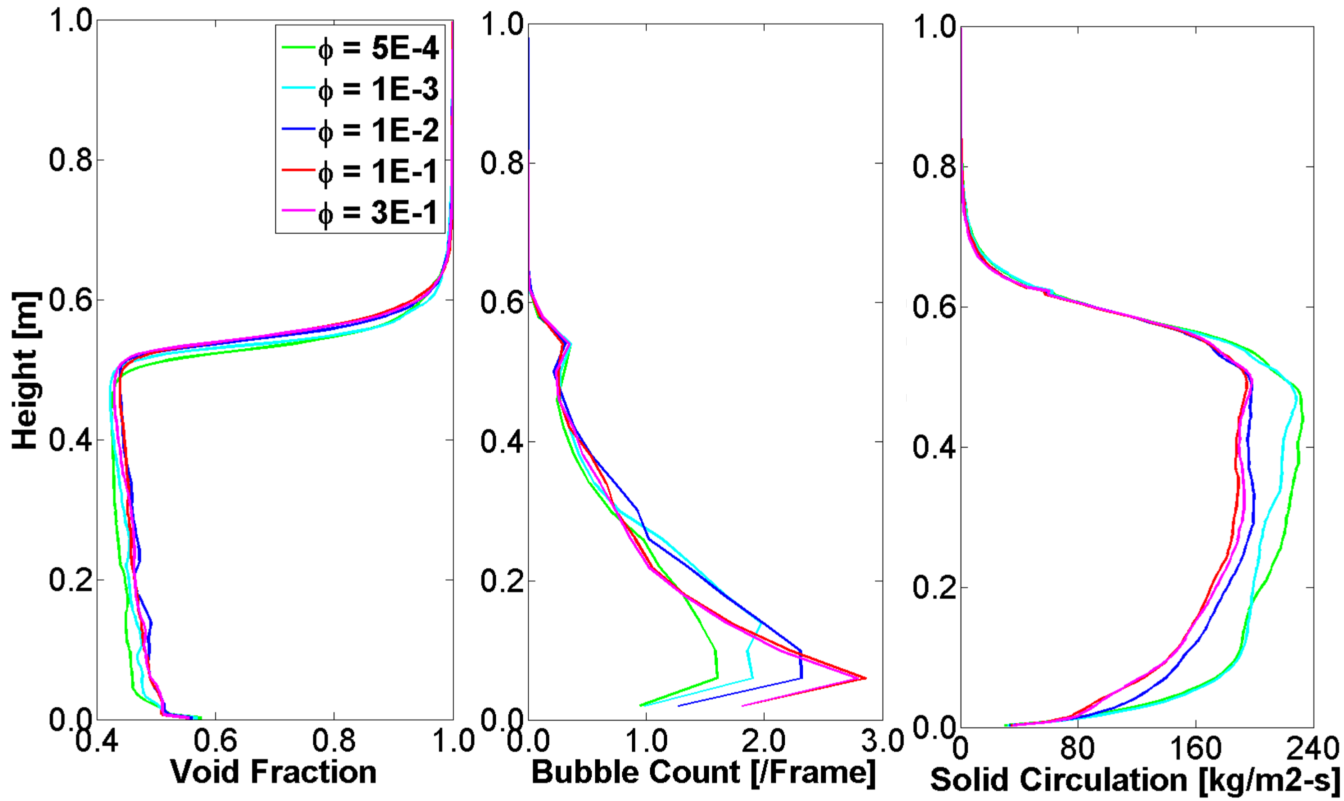
$$t_c|_{y_1} = t_c^+|_{y_1} + t_c^-|_{y_1} = \int_0^{y_1} \Delta t_c^+(y) + \Delta t_c^+(y)\,dy$$





Pilot-Scale Cylindrical Bed

- Cylindrical grid - 40x200x20 for 30 cm bed (average dr = 12 d_p)
- Time mean pressure and void fraction profiles show negligible differences
- **Circulation flux about 25% higher for lower ϕ**



Influence of φ on flow metrics for cylindrical bed with diameter = 30 cm and U = 4.6 U_{mf} (18.9 cm/s)

Lab-Scale Cylindrical Bed

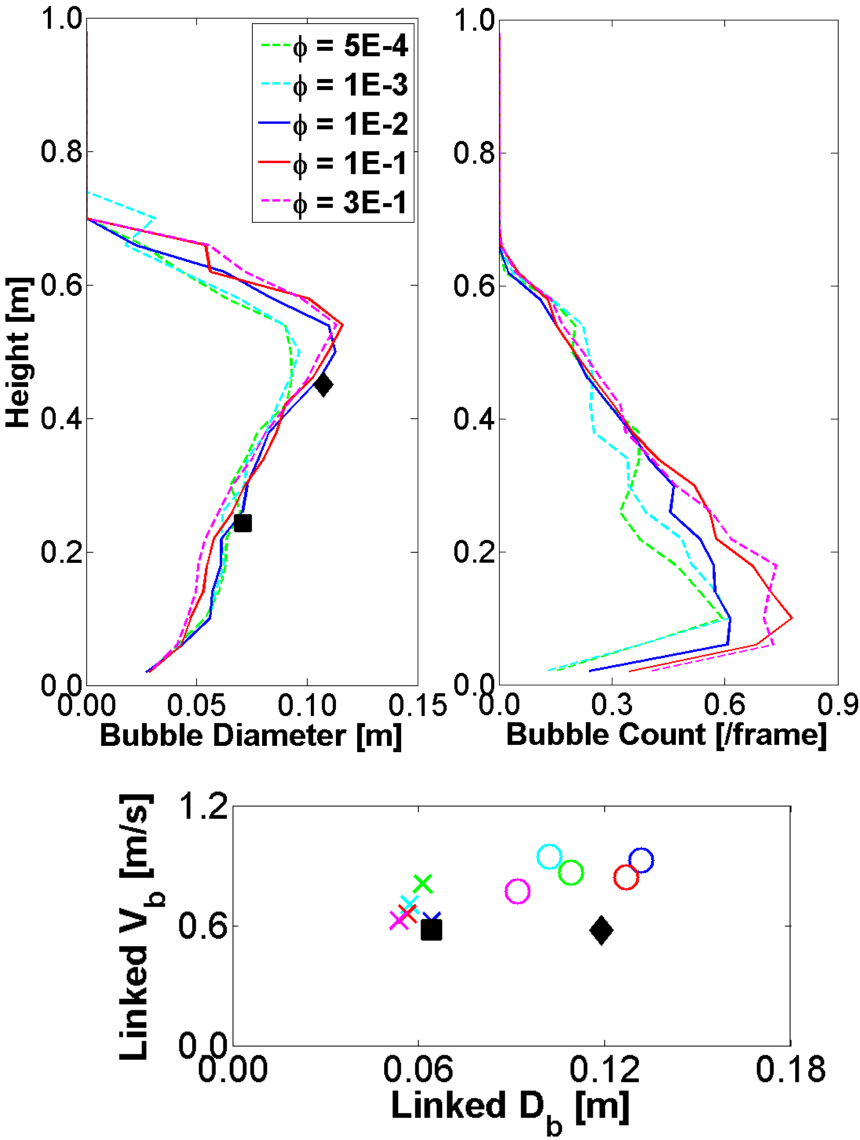
Choosing Φ

Bubble Diameter Predictions

- Only bubbles within 2.5 cm from bed axis counted to replicate experiments
- Better agreement between experiment and simulation for $\varphi \in [0.01, 0.1]$

Bubble Velocity Predictions

- About 10% of bubbles detected are linked (based on filters on bubble position, velocity)
- Good agreement at lower probe (*filled square*)
- Difference at upper probe (*filled diamond*) due to formation of slugs, experimental standard deviation + cross-correlation function



Conclusions and Future Work

i. **Circulation flux and bubble statistics** must supplement time mean solid holdup and pressure profiles to quantify hydrodynamics and mixing
ii. Wall boundary condition is critical for simulating fluidization and may even impact predictions in pilot-scale simulations
iii. Studies on both thin rectangular bed and cylindrical beds indicate appropriate specularity coefficient for bubbling fluidization in the range **0.01-0.1**

Future Work

i. Validation with different experimental setup / particle size / flow parameters
ii. Experimental data to quantify circulation time for cylindrical beds
iii. Using bubble statistics to predict residence times in reactive simulations

References

[1] Johnson, P.C. and Jackson, R. "Frictional-collisional constitutive relations for granular materials, with application to plane shearing." *J. Fluid Mech.* 176 (1987): 67–93.

[2] Sánchez-Delgado, S. et al. "Estimation and Experimental Validation of the Circulation Time in a 2D Gas–solid Fluidized Beds." *Powder Technology* 235.0 (2013): 669–676.

[3] Rüdisüli, Martin et al. "Comparison of Bubble Growth Obtained from Pressure Fluctuation Measurements to Optical Probing and Literature Correlations." *Chemical Engineering Science* 74.0 (2012): 266–275.

[4] Bakshi, A., C. Altantzis, and A.F. Ghoniem. "Towards Accurate Three-dimensional Simulation of Dense Multi-phase Flows Using Cylindrical Coordinates." *Powder Technology* 264.0 (2014): 242–255.

[5] Altzantis, C., R. B. Bates, and A.F. Ghoniem. "3D Eulerian modeling of thin rectangular gas-solid fluidized beds: Estimation of the specularity coefficient and its effects on bubbling dynamics and circulation times." *Submitted to Powder Technology (2014)*.