Experimentation, CFD and Reactor Models: Complementary Tools for Resolving Challenging Issues in Fluidization

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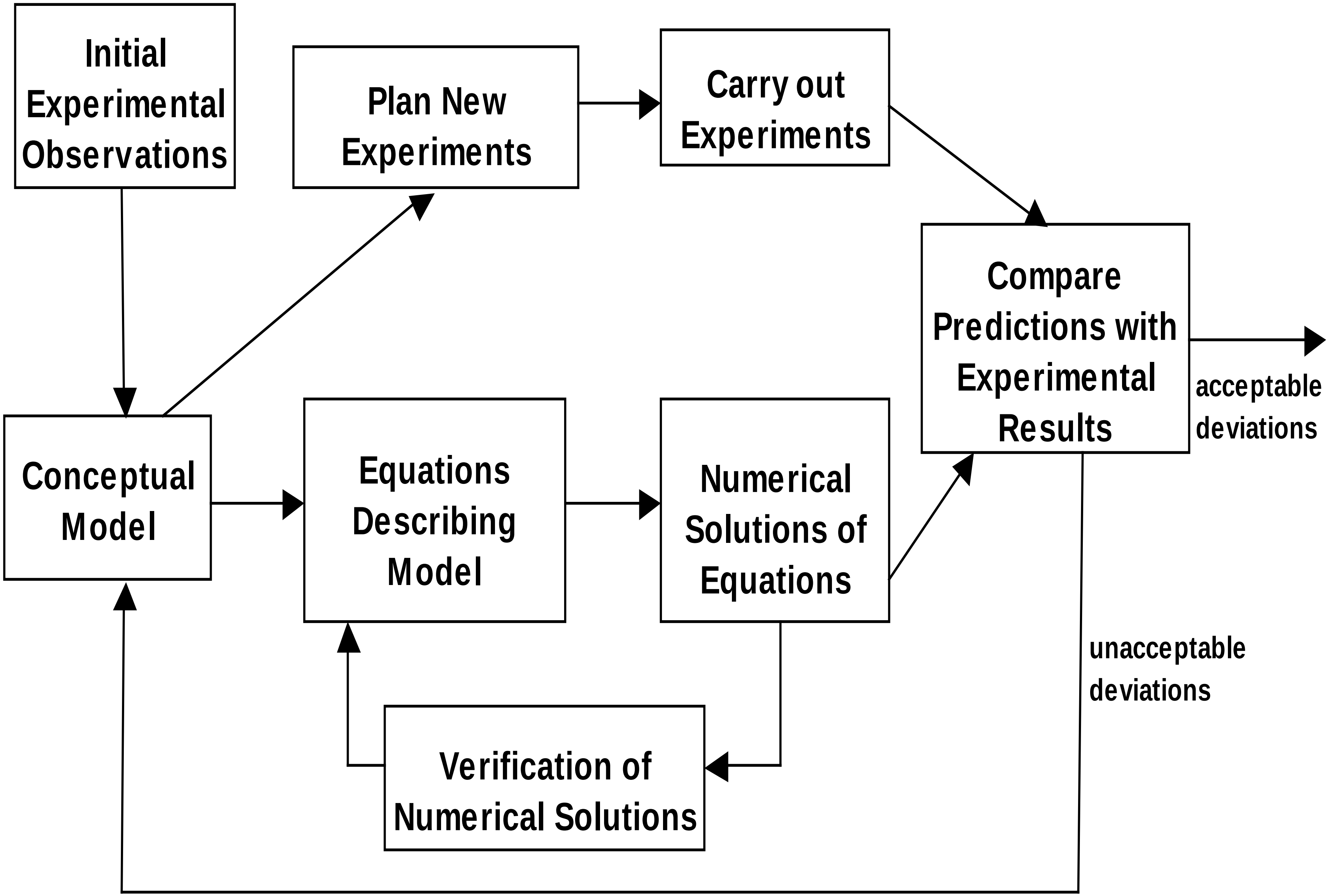
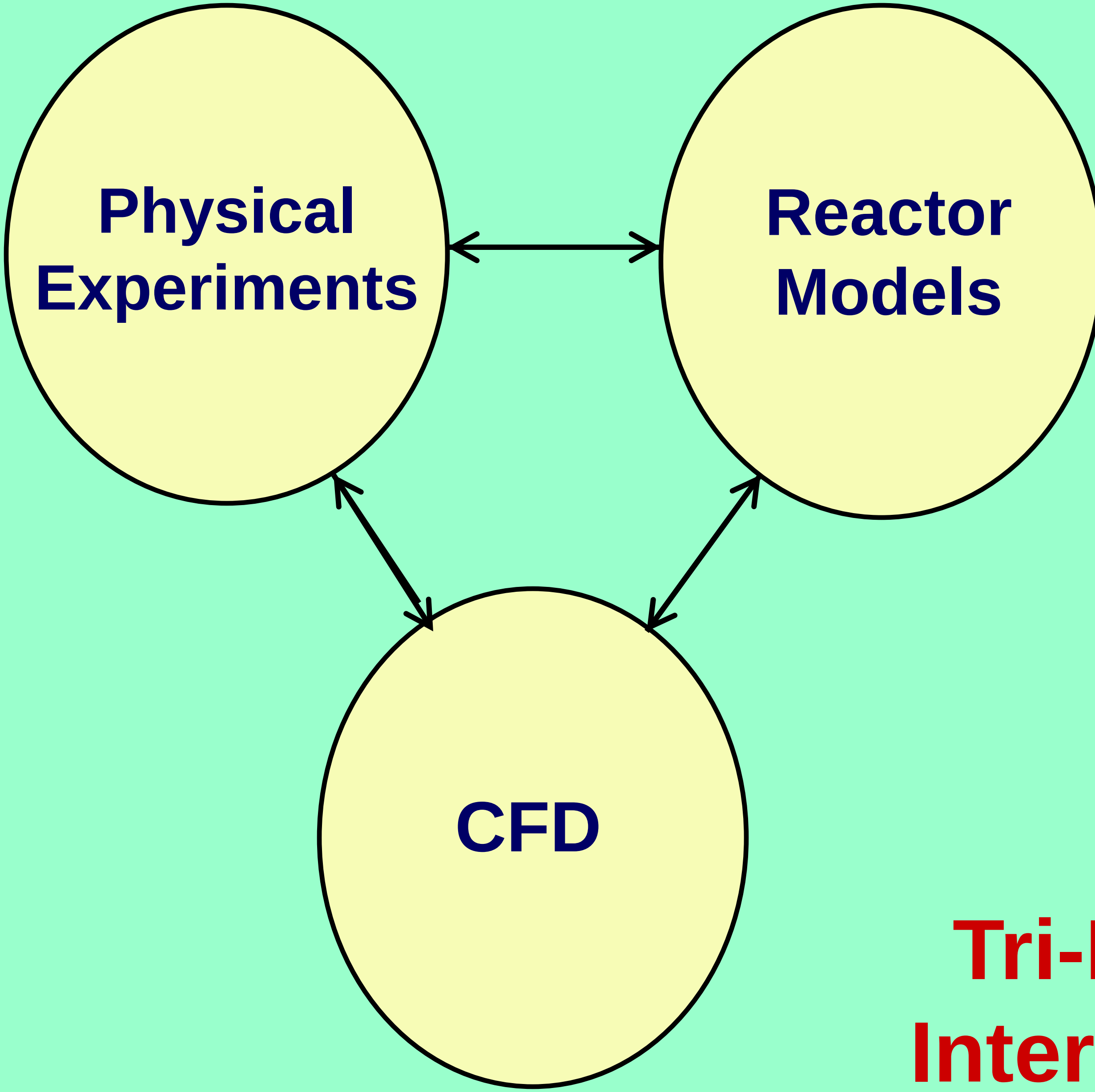
Key Steps in Building and Validating Models



Background

It is well understood, though not always acted on, that experimental validation is essential for successful application of CFD codes to difficult multiphase flows like fluidized beds.

This presentation will attempt to outline some cases where the interaction can potentially go further, providing information that otherwise would be virtually impossible to gather.



Tri-Partite Interactions

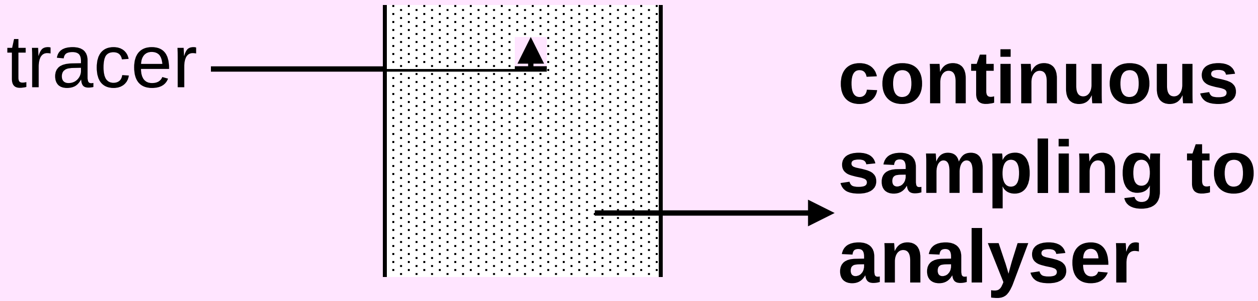
Hierarchy of Fluid Bed Reactor Models

Type	**Model Complexity**
Purely empirical correlations	Simple; may even lack dimensional consistency
Empirical correlations based on dimensional analysis	Usually involves multi-variate regression.
Semi-empirical: mechanistic plus fitted constant(s)	Usually results in explicit equation or equations.
Physical “cold models” for dynamically similar expts.	Requires geometric scaling and matching of Π groups
Fully mechanistic models	Requires solution of set of DEs or algebraic eqns.
Comprehensive models based on physical laws, balances	Numerical solution, e.g. via CFD codes

1. Experimental Evidence from Axial Gas Mixing Related to Wall Particle Slip Boundary Condition

- Gas backmixing in fluidized beds is important in determining the conversion and selectivity in fluidized bed reactors.

- It is often measured experimentally using a tracer (e.g. helium) injected at one level and then detected upstream:

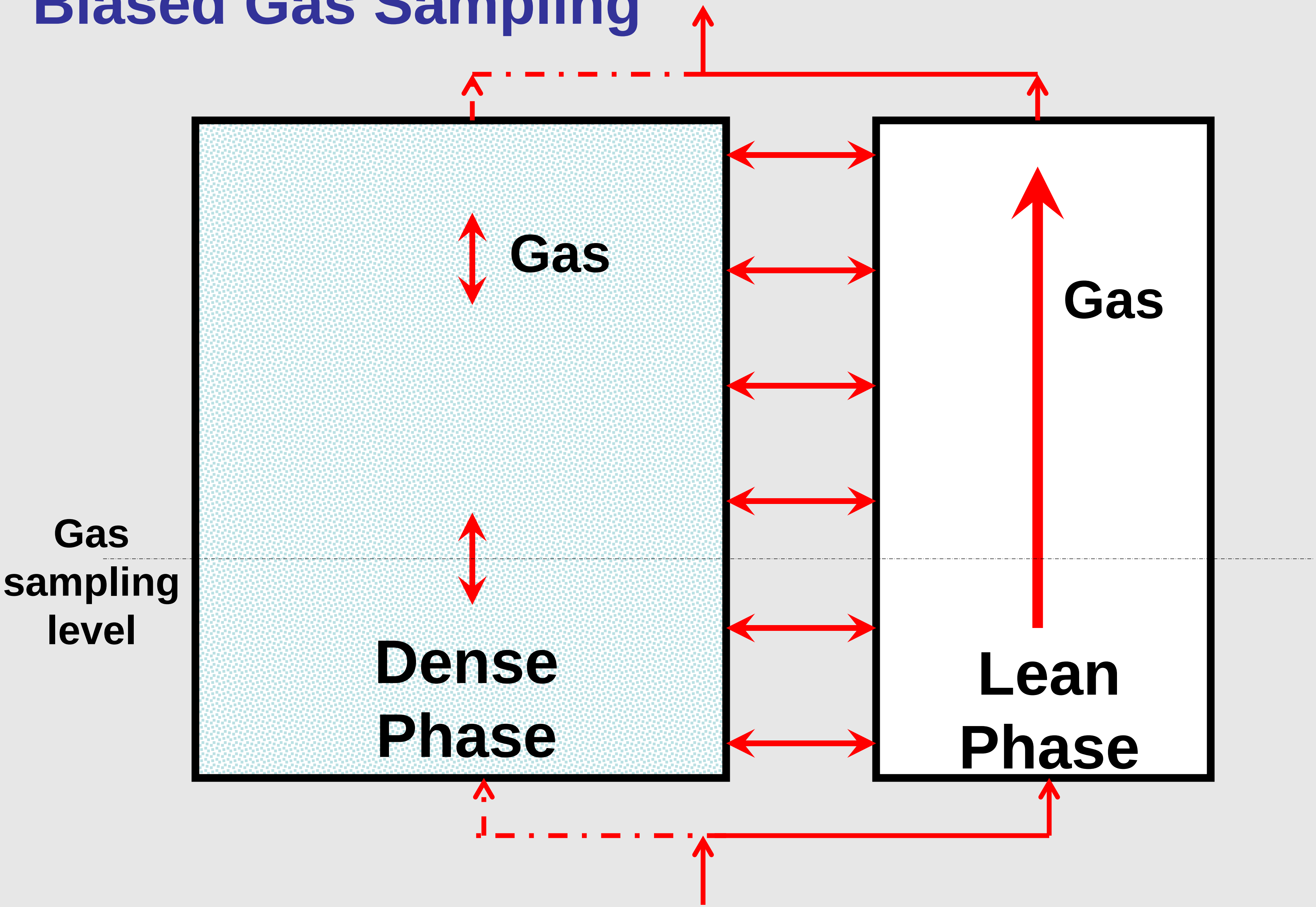


Axial Gas Mixing in Fluidized Beds

- Consider a steady state back-mixing test as shown below.
- Gas backmixing in fluidized beds is caused by drag by particles descending near the outer walls.
- Commonly this is modelled (erroneously) as axial dispersion (diffusion-like process).

Li Tingwen, Zhang YM, Grace JR and Bi XT, Numerical investigation of gas mixing in gas-solid fluidized beds, AIChE Jl., in press.

Biased Gas Sampling



Grace JR, Bi XT and Zhang YM, Pitfalls in gas sampling from fluidized beds, Chem. Eng. Sci., 64, 2522-4 (2009).

Askins et al, CEP, 1951

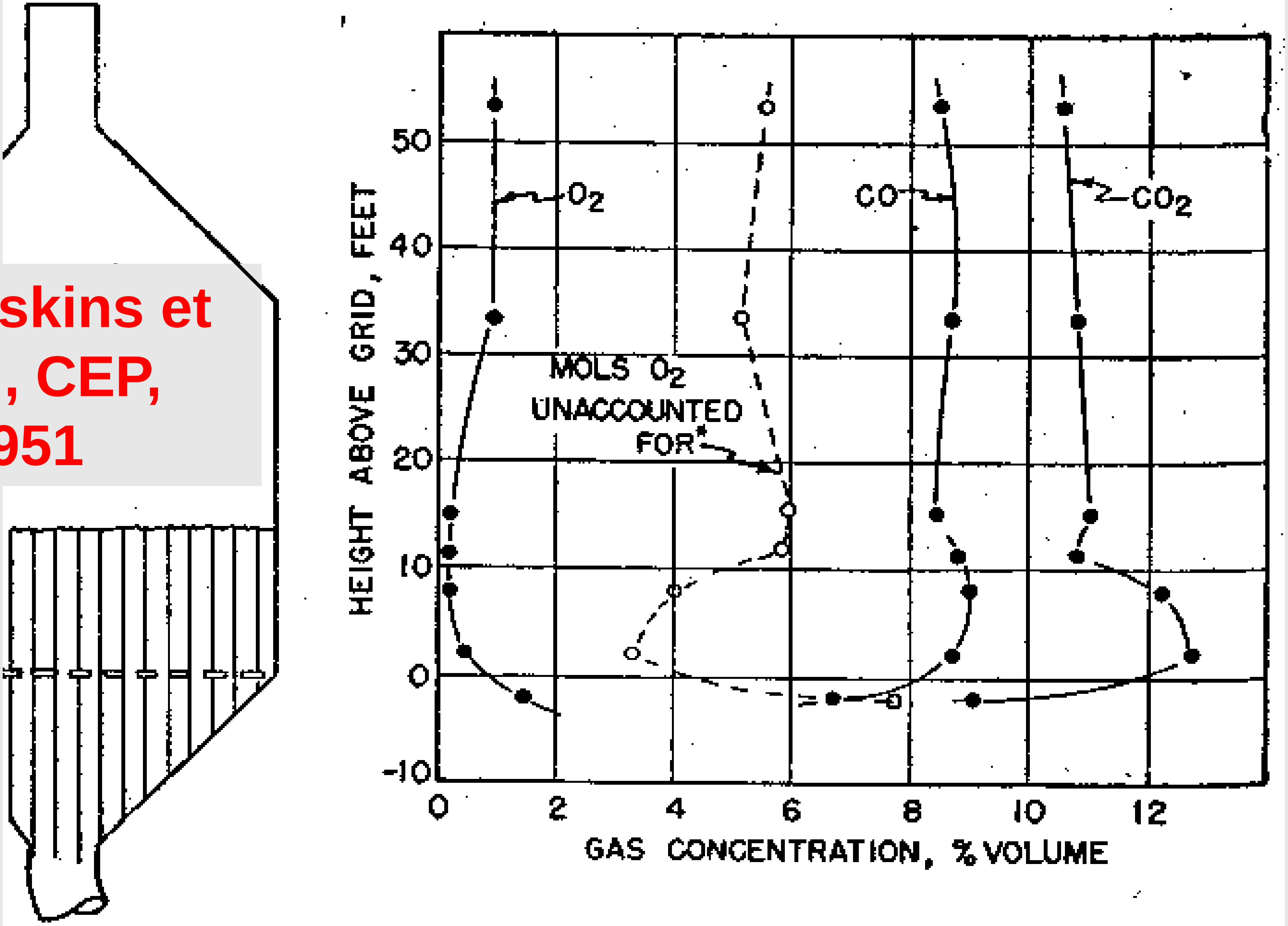


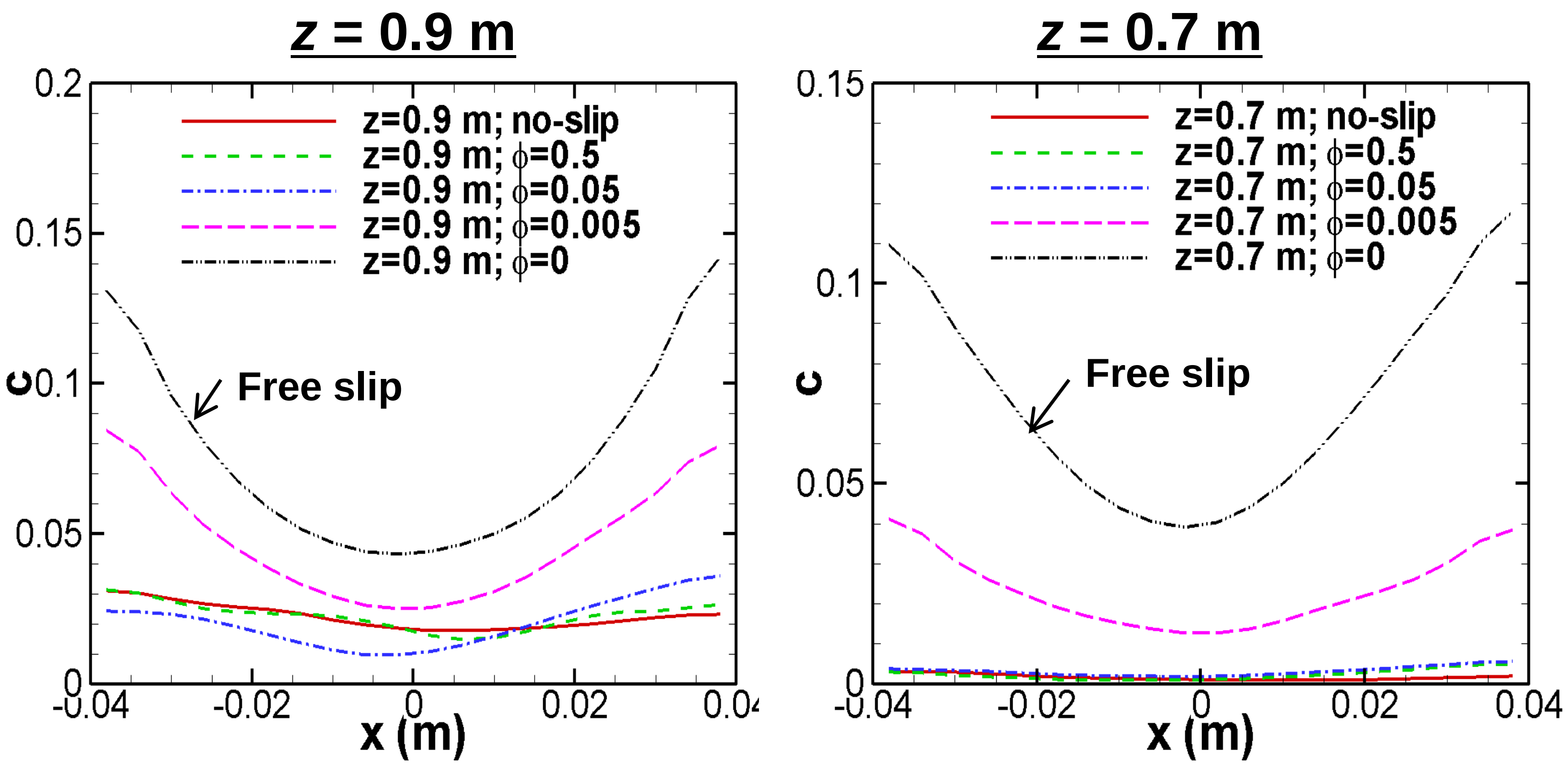
Fig. 5. Vertical gas concentration profile of regenerator.
* Same numerical scale as gas concentration.

Physical System Modelled

76 mm i.d. x 1.830 m tall column studied by Mason (1950) with 155 µm glass beads and helium tracer injected at z = 1.05 m

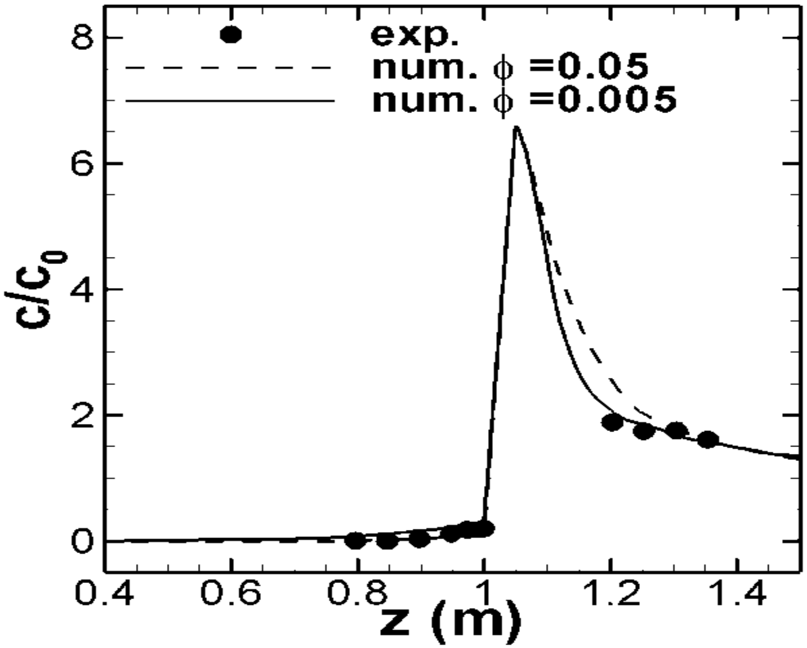
- CFD Eulerian-Eulerian model
- Kinetic granular theory
- 3-D simulation, ~100,000 grid points
- Fluent 6.3
- Little influence of coefficient of restitution or turbulent diffusivity.
- Johnson & Jackson partial slip B.C. at wall.

Effect fo Wall B.C. on Backmixing

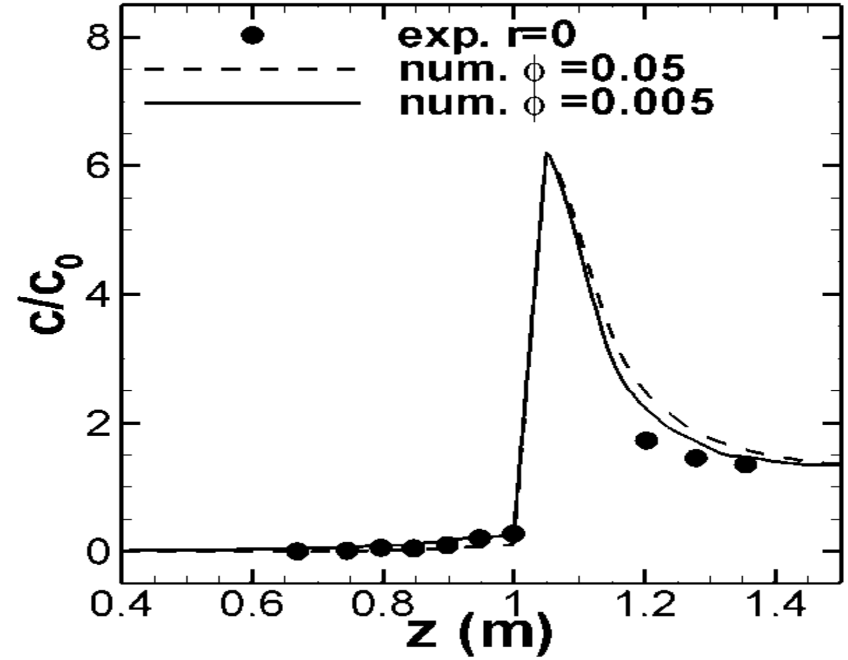


Influence of specularity coefficient on lateral profiles of upstream tracer concentration: 2-D simulations

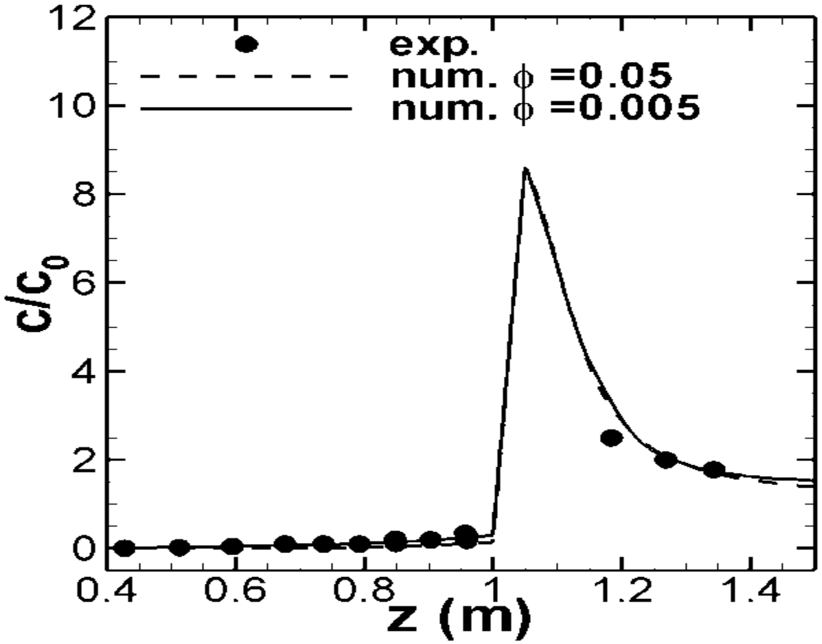
(a)



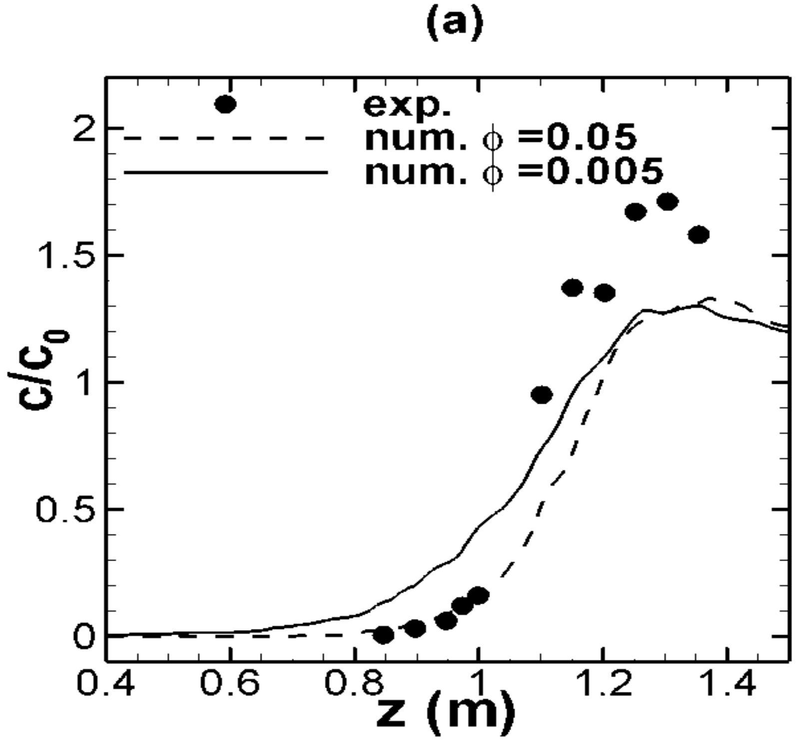
(b)

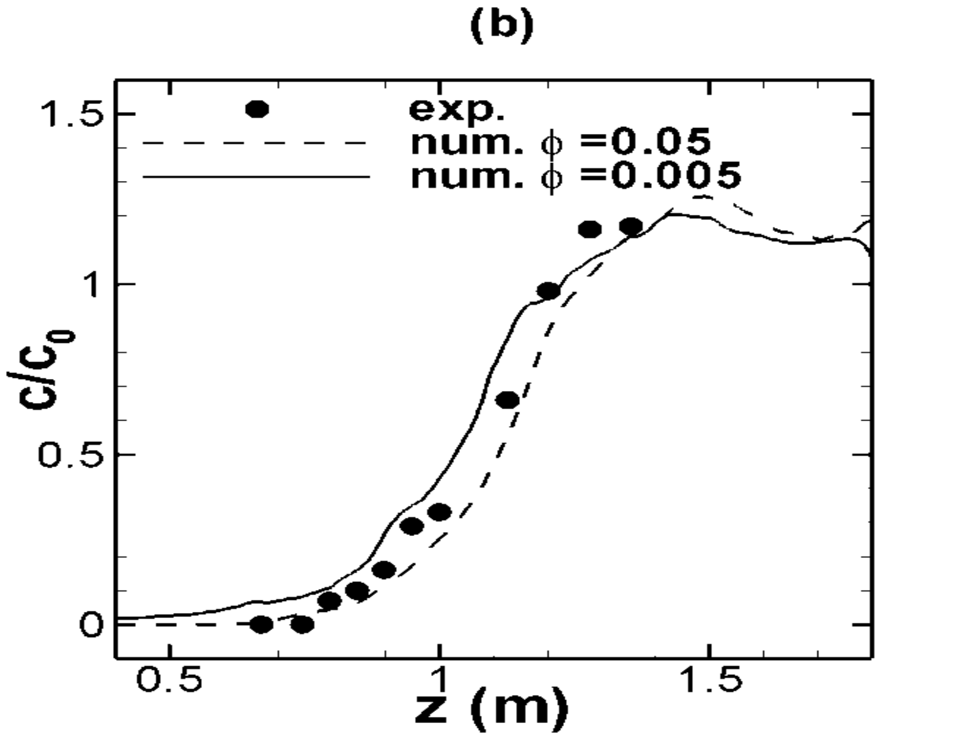


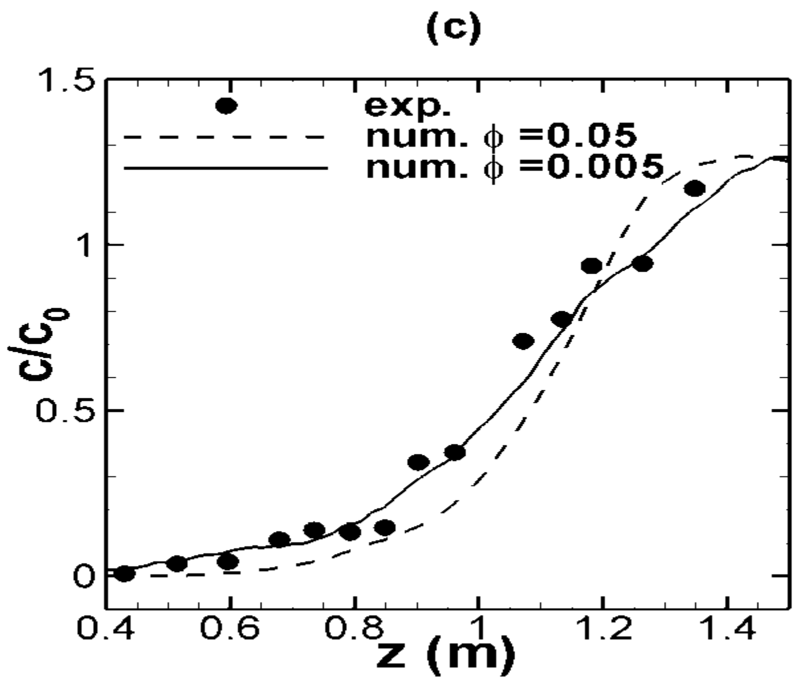
(c)



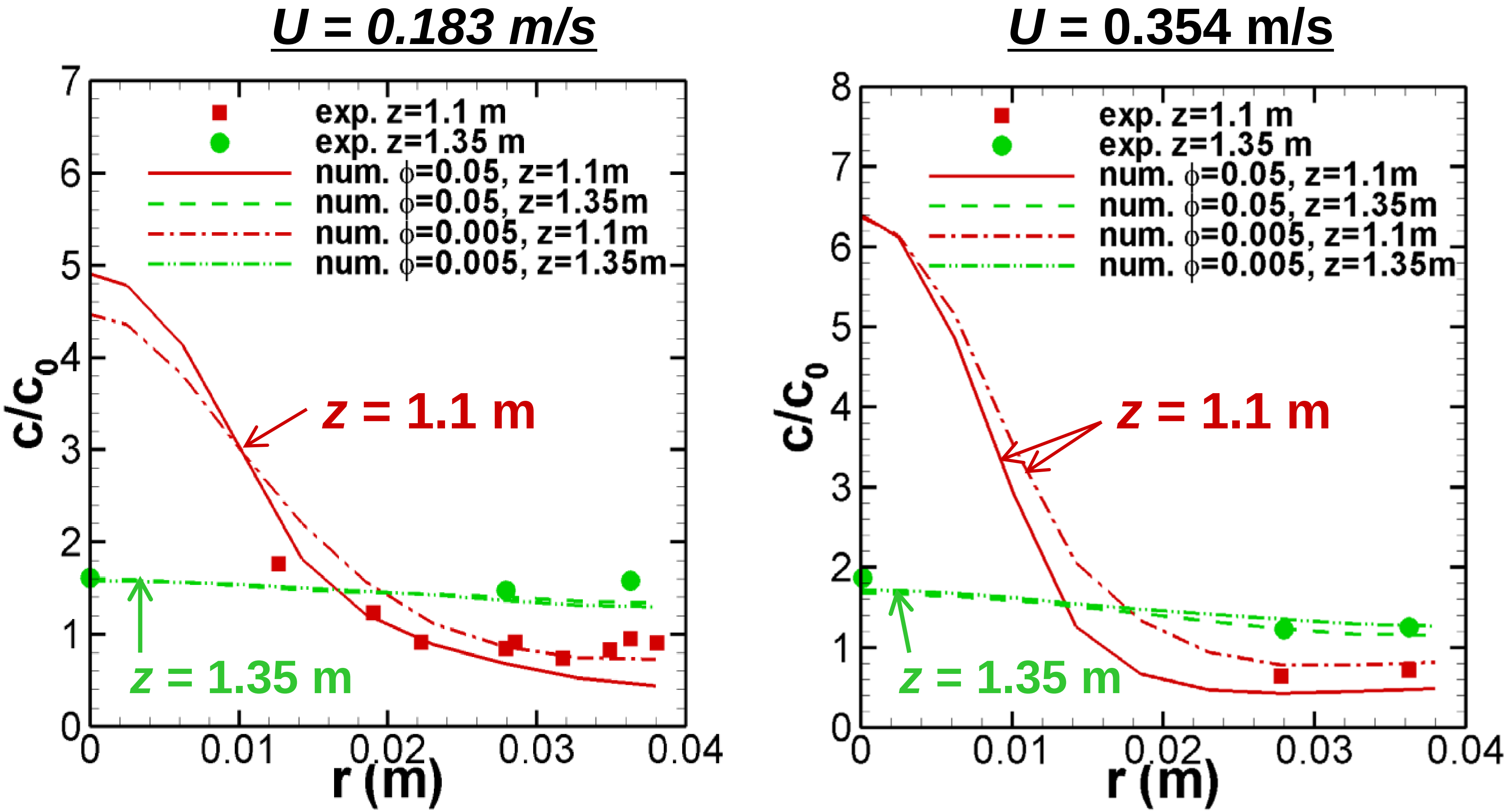
Axial profiles of mean tracer concentration predicted by 3-D simulations **at *r* = 0** for U_g= (a) 0.183 m/s; (b) 0.274 m/s; (c) 0.354 m/s



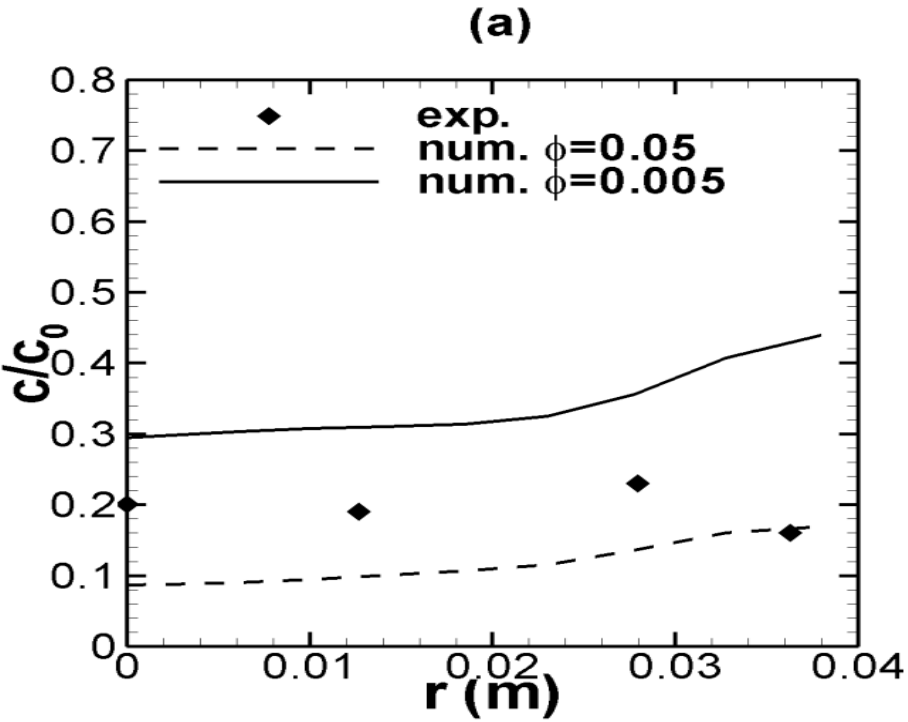


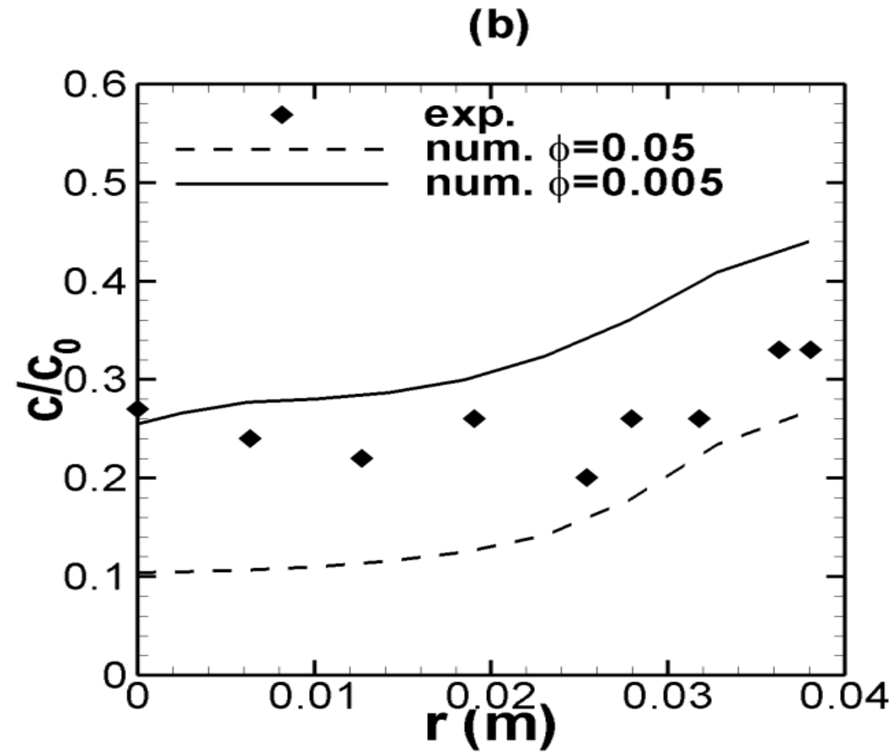


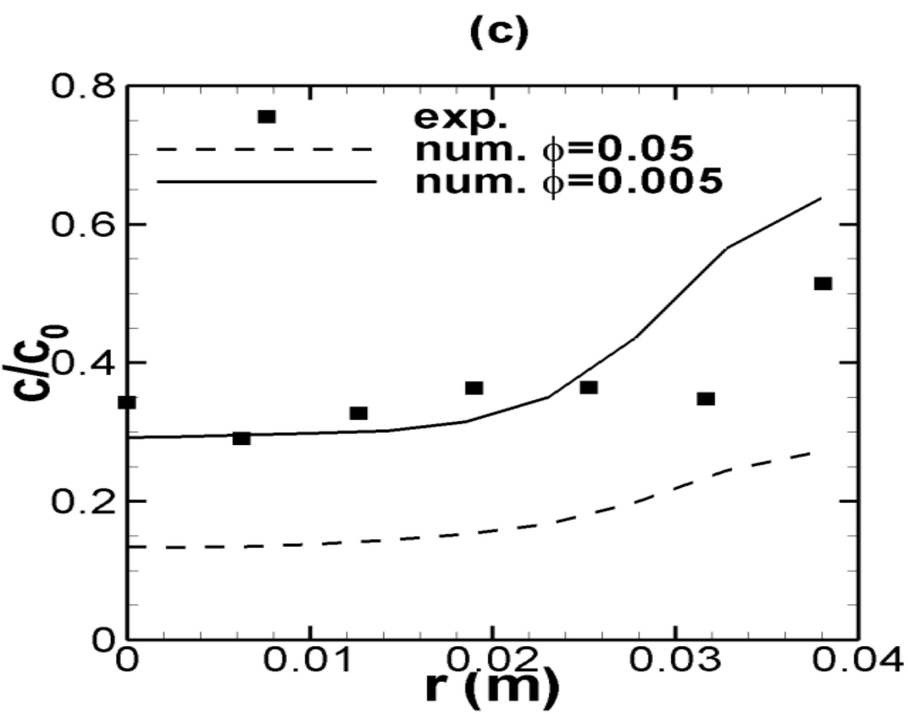
Axial profiles of mean tracer concentration predicted by 3-D simulations at ***r* = 36 mm** for U_g= (a) 0.183 m/s; (b) 0.274 m/s; (c) 0.354 m/s.



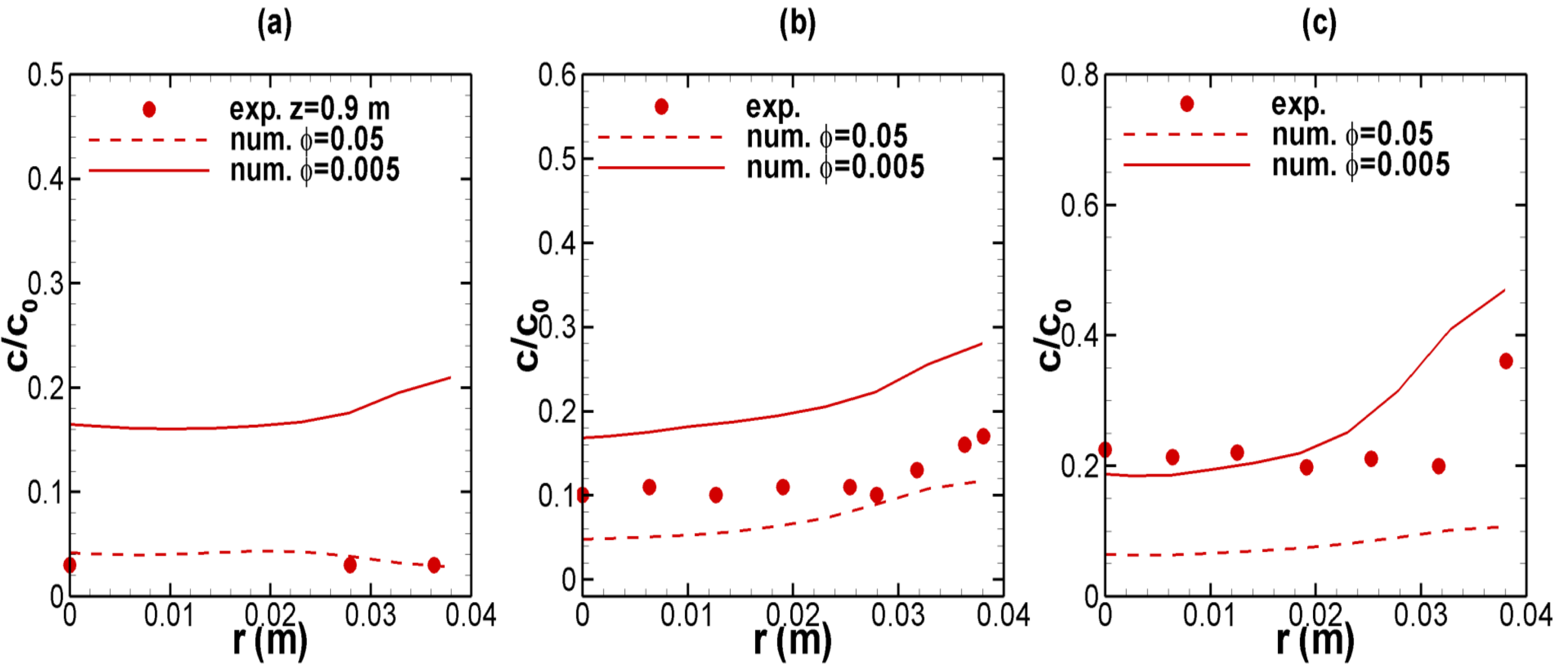
Radial profiles of mean tracer concentration above injection level







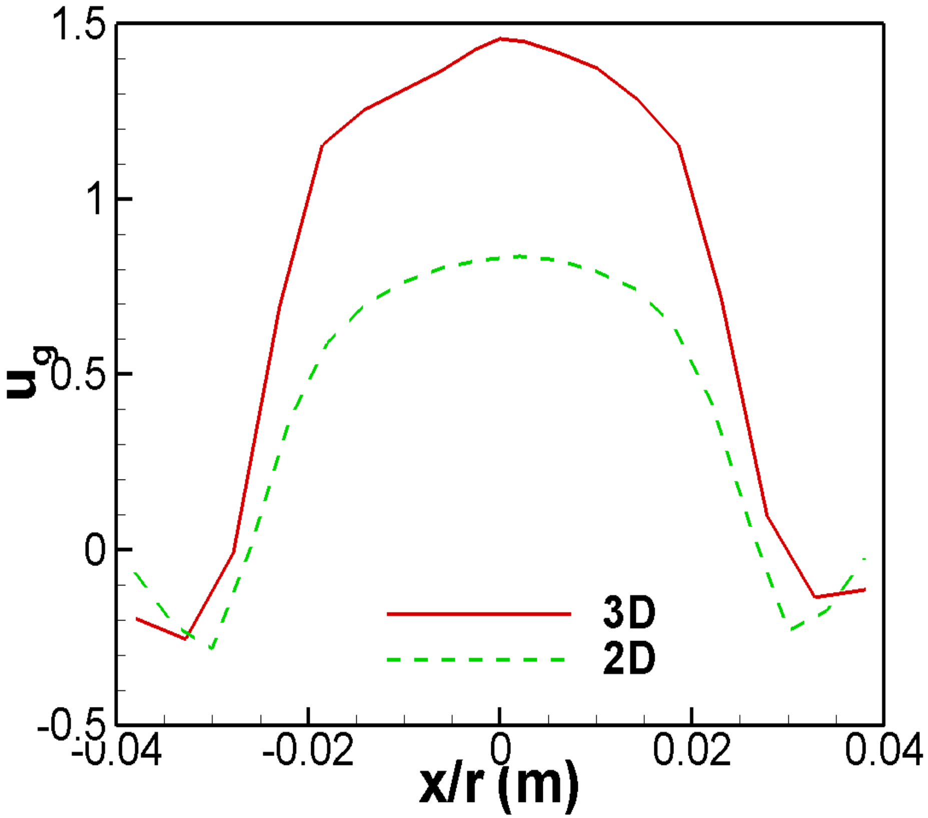
Radial profiles of mean tracer concentration at <u>**z = 1.0 m**</u> for U_g= (a) 0.183 m/s; (b) 0.274 m/s; (c) 0.354 m/s.



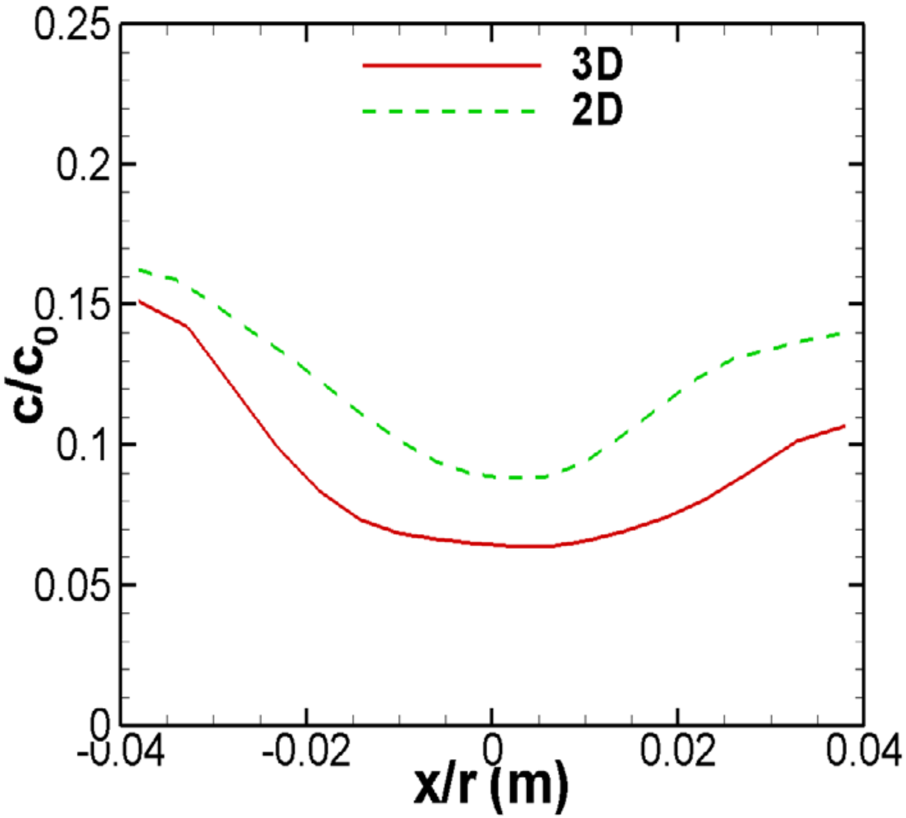
Radial profiles of mean tracer concentration at *z* = 0.9 m for U_g= (a) 0.183 m/s; (b) 0.274 m/s; (c) 0.354 m/s.

2-D vs 3-D Simulations

Vertical gas velocity profile



Tracer concentration profile



Radial profiles of time-average gas vertical velocity and tracer concentration by 2-D and 3-D simulations.

Parametric Studies

2-D simulations were used to conduct parametric studies

- Bed height
- Tracer flow rate
- Particle-particle restitution coefficient
- Turbulence diffusivity
- Wall boundary condition

Lesson: Solid-phase wall boundary condition needs to be specified with great care when modelling mixing. Free slip, partial slip and no-slip boundary conditions give substantially different gas backmixing.

Summary: Effect of Wall B.C.

- Specularity coefficient has a significant impact on the flow hydrodynamics near the wall.
- Since gas backmixing is initiated by drag of the descending particles at the wall, it is sensitive to the specularity coefficient in the range 0 to 0.05.
- Experimental backmixing measurements may then provide a means of specifying the specularity coefficient.

2. How Representative are Two-Dimensional Fluidized Beds?

- Thin fluidized beds, commonly referred to as “two-dimensional”, are often used both as educational tools and to gain quantitative information that might help understand the behaviour of fully three-dimensional columns.
- The idea is that should provide a view of a slice through a fully 3-D column.
- How “two-dimensional” are they?
- Also relevant to the question of whether 2-D simulations can be used for real 3-D columns.

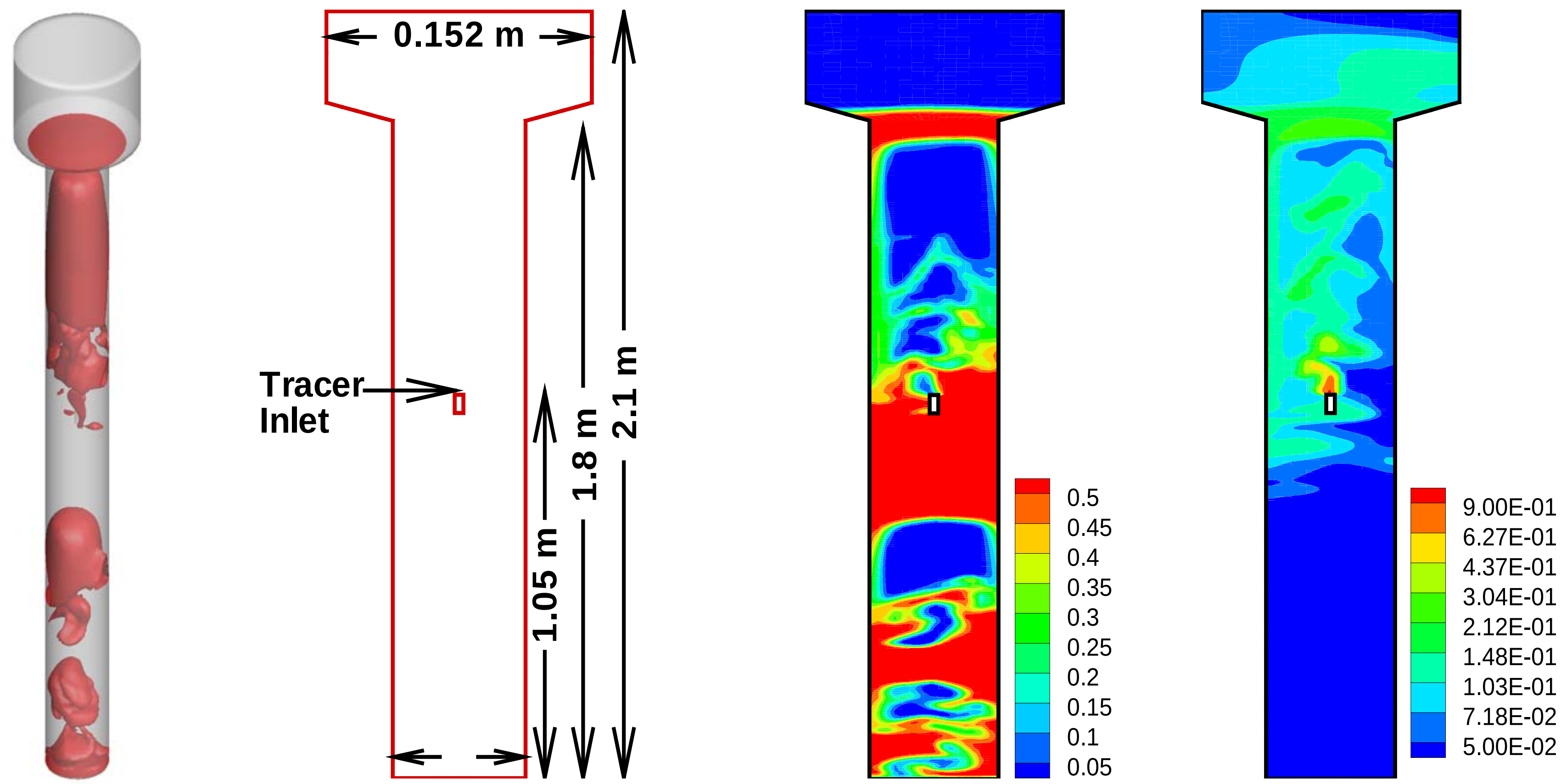
Experiment & Simulation Set-up

- Experiment
  - 2-D bubbling fluidized bed of Laverman et al. 2008
  - Geometry: 0.3 x 0.7 x 0.015 m; U = 0.27 & 0.45 m/s
  - Mean particle diameter: 485 µm
- Simulation:
  - MFIX
  - Johnson and Jackson (1987) B.C.s
  - e_w = 0.95; φ = 0, 0.005, 0.05, 0.5

Laverman, J. A.; Roghair, I.; Annaland, M. V.; Kuipers, H., Investigation into the hydrodynamics of gas-solid fluidized beds using particle image velocimetry coupled with digital image analysis. *Can J Chem Eng* **2008,** 86, (3), 523-535.

Numerical Simulation cont'd

- Simulation setup and results

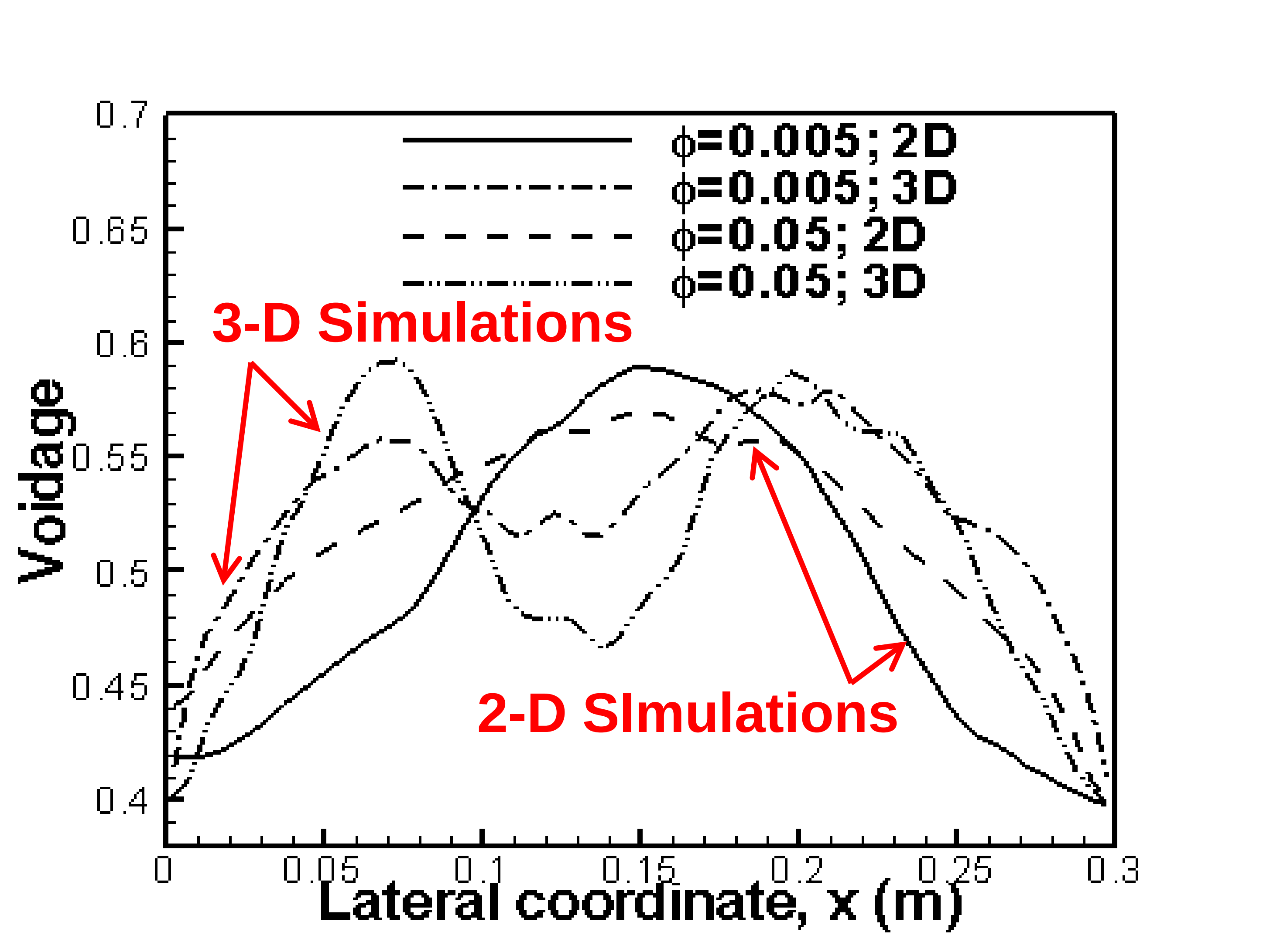


Domain schematic

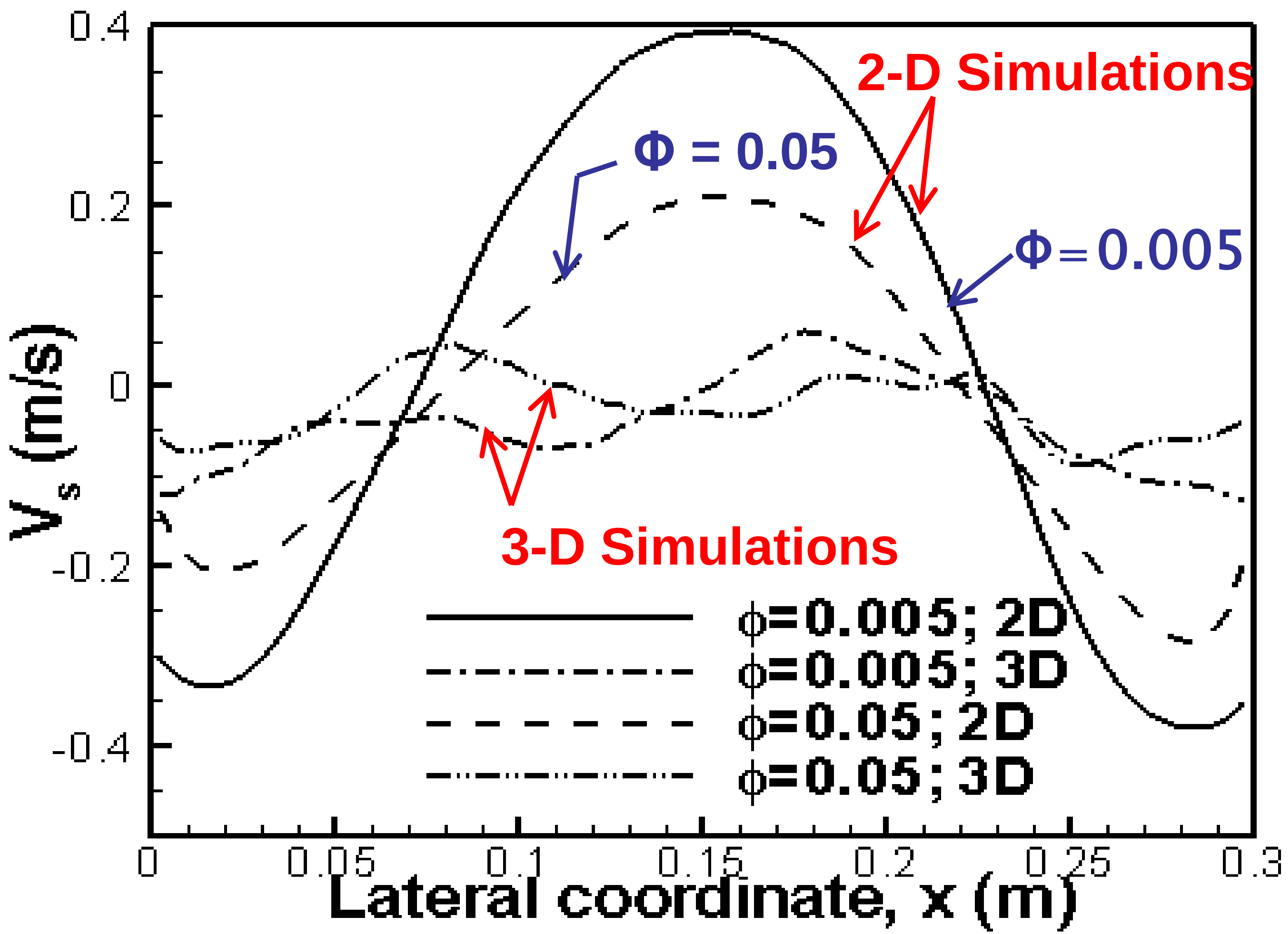
Solid volume fraction

Tracer mole fraction

3-D Simulation of 2-D Column



Lateral profile of time-mean voidage at z = 0.2 m for $U_g = 2.5U_{mf}$ predicted by 2-D and 3-D simulations. Simulation time: 70 s for 2-D; 10 s for 3-D.



Lateral profile of time-mean vertical solid velocity at *z* = 0.2 m for $U_g = 2.5 Umf$ predicted by 2-D and 3-D simulations. Simulation time: 70 s for 2-D; 10 s for 3-D.

Bubble Diameter Averaging Methods

Equivalent bubble diameter:

- Diameter average:

$$\bar{D}_{b,eq} = \sum D_{b,eq} \big/ N \qquad D_{b,eq} = \sqrt{4A/\pi}$$

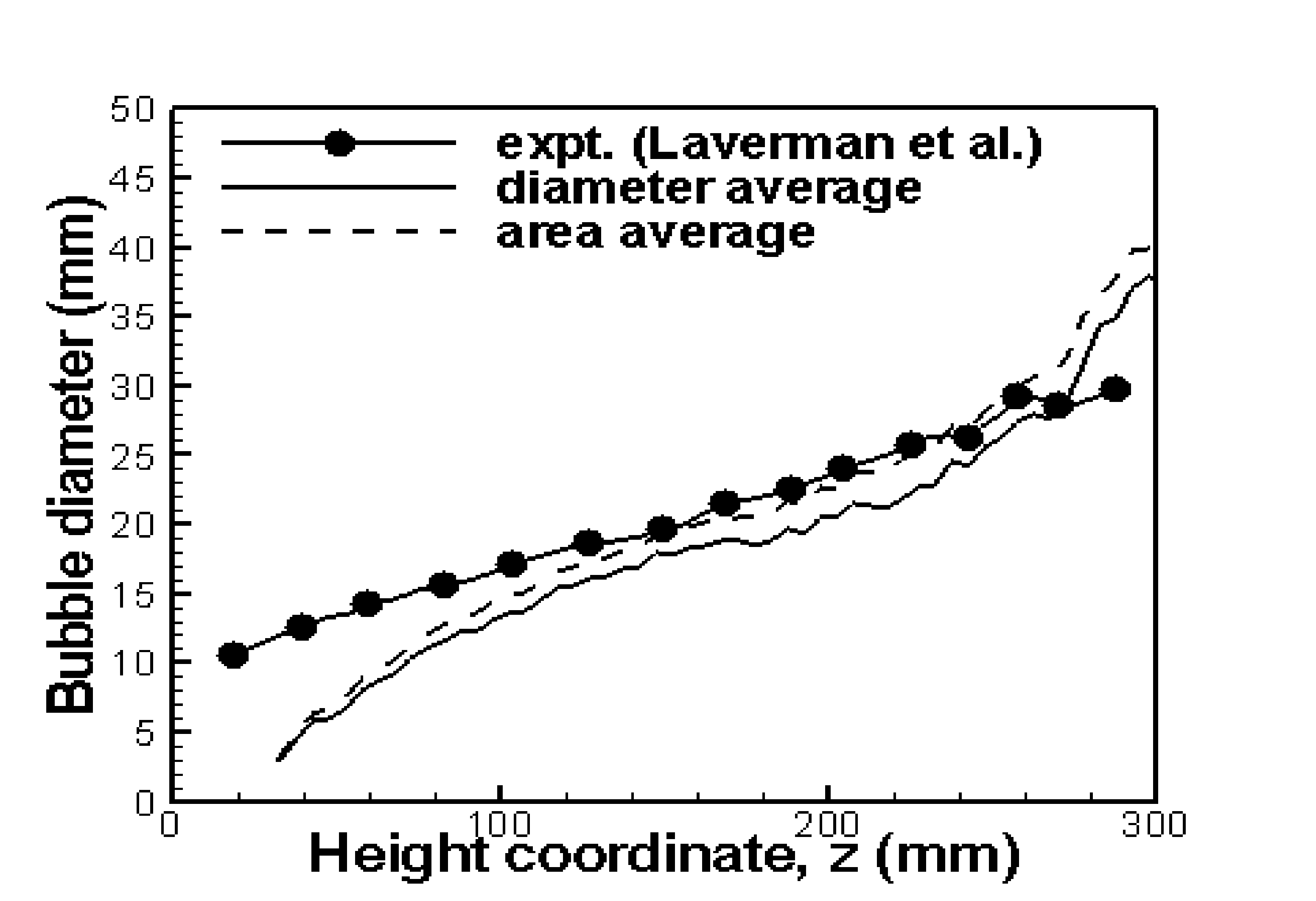
- Area average:

$$\bar{D}_{b,eq} = \sqrt{4\bar{A}/\pi} \qquad \bar{A} = \sum A \big/ N$$

where *A*: void frontal area

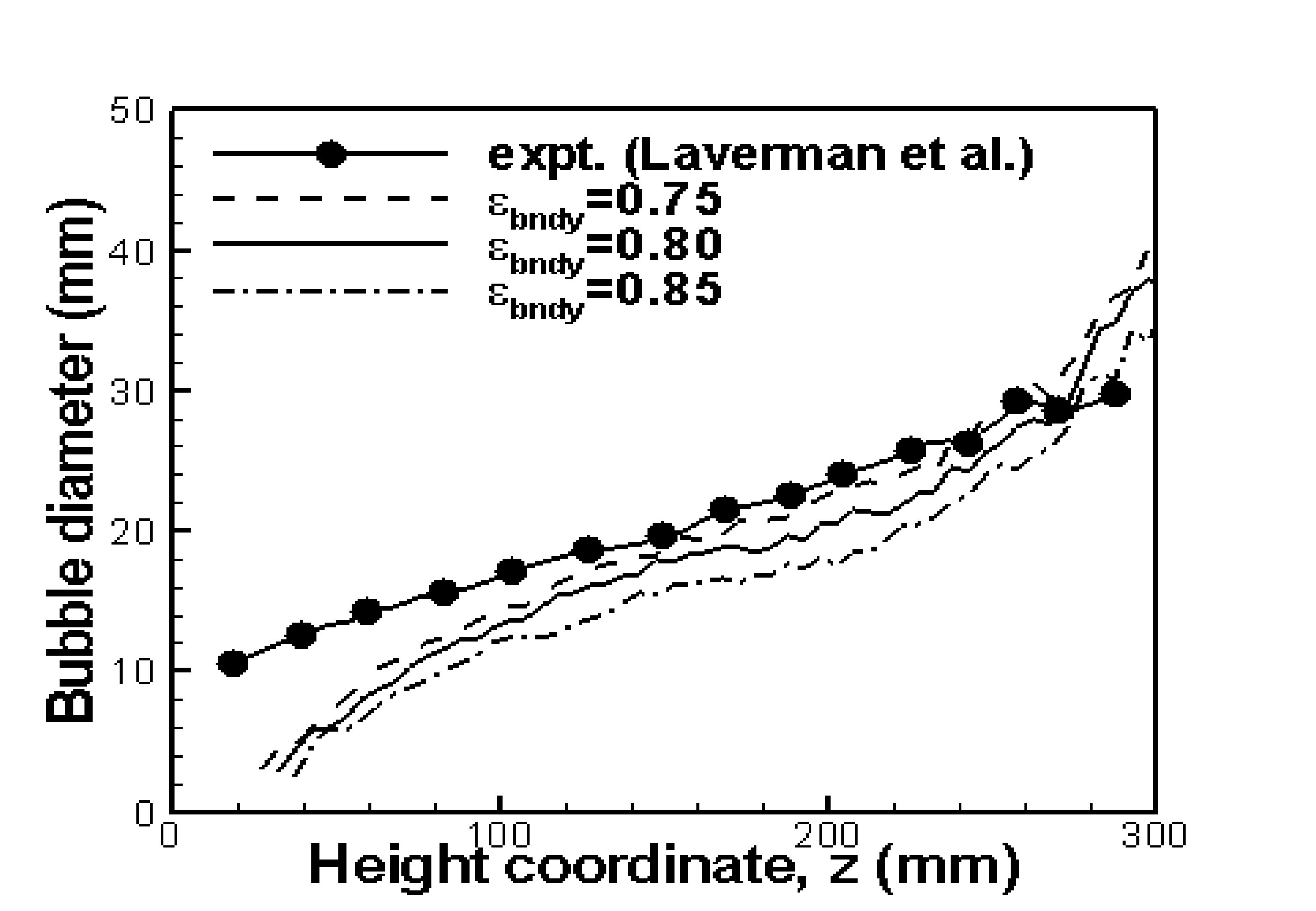
and *N*: total bubble number.

Effect of Averaging Method



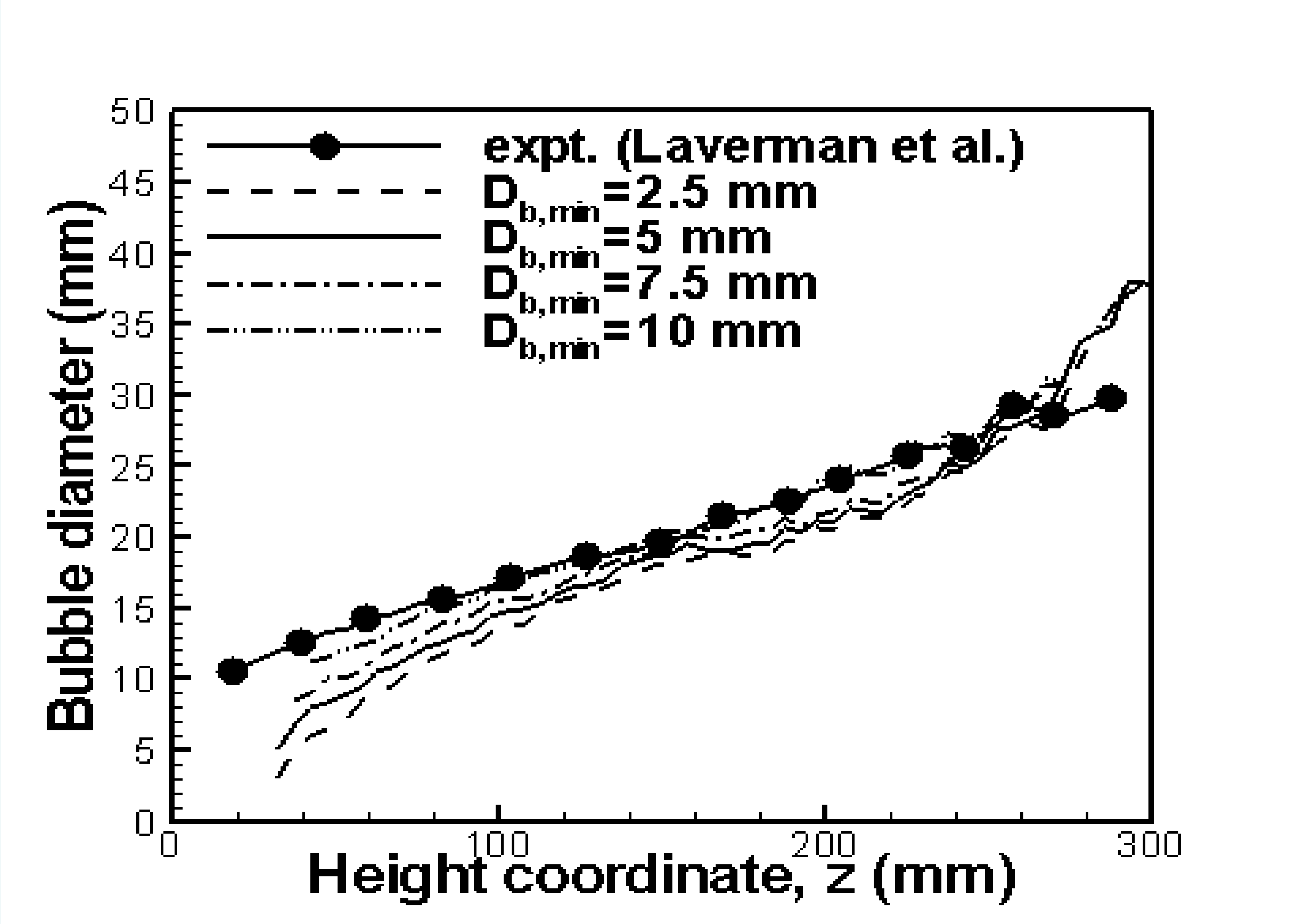
Mean bubble diameters calculated by two methods: U_g=1.5U_{mf}; e_w= 0.8; ϕ= 0.05; $D_{b,min}$= 2.5mm; 3-D simulation.

Effect of Bubble Boundary



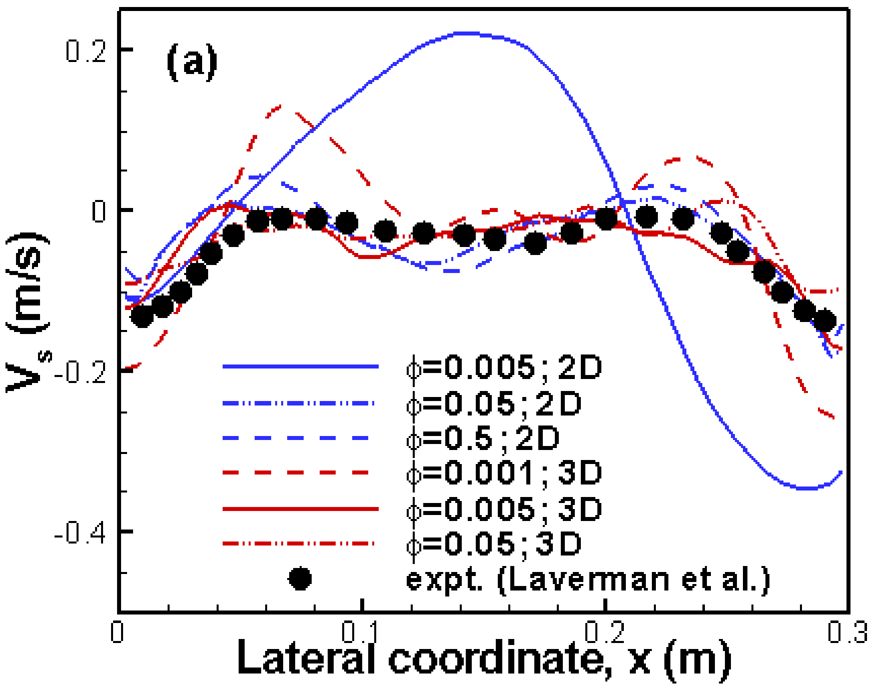
Mean bubble diameters calculated with different bubble definitions (U_g=1.5 U_{mf}; $\Phi = 0.05$; $D_{b,min}$ = 2.5 mm; 3-D simulation).

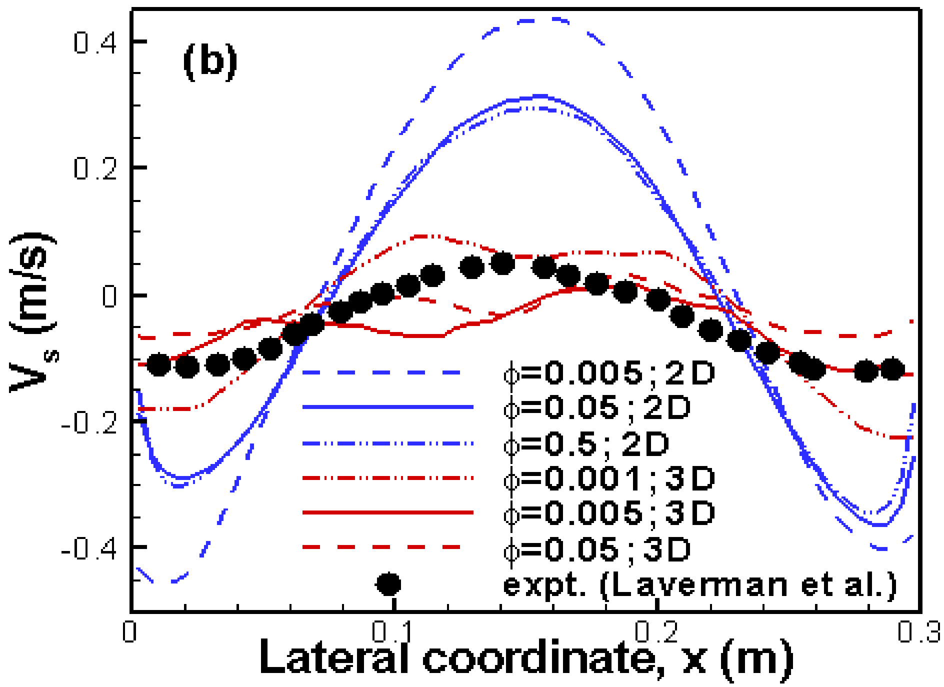
Effect of Minimum Bubble Diameter



Mean bubble diameter calculated with different minimum bubble sizes (U_g=1.5U_{mf}; ϕ = 0.05; ε_{bndy} = 0.8; 3-D simulation).

Comparison with Experimental Particle Velocity



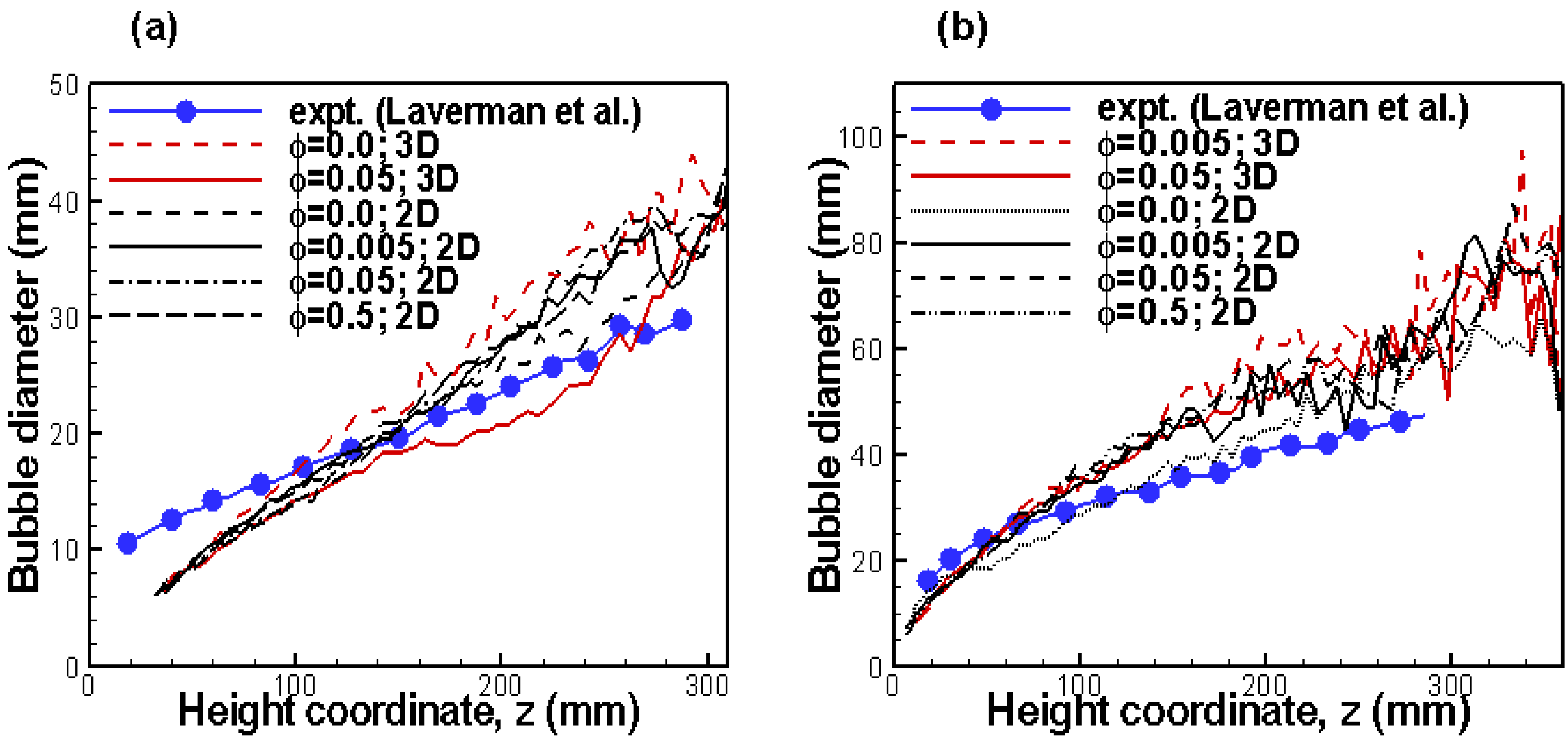


Lateral profiles of time-mean solid velocity at (a) z = 0.105 m; (b) z = 0.245 m for U_g=2.5U_{mf}.

Red: 3-D SImulations

Blue: 2-D Simulations

Comparison with Experimental Bubble Diameters

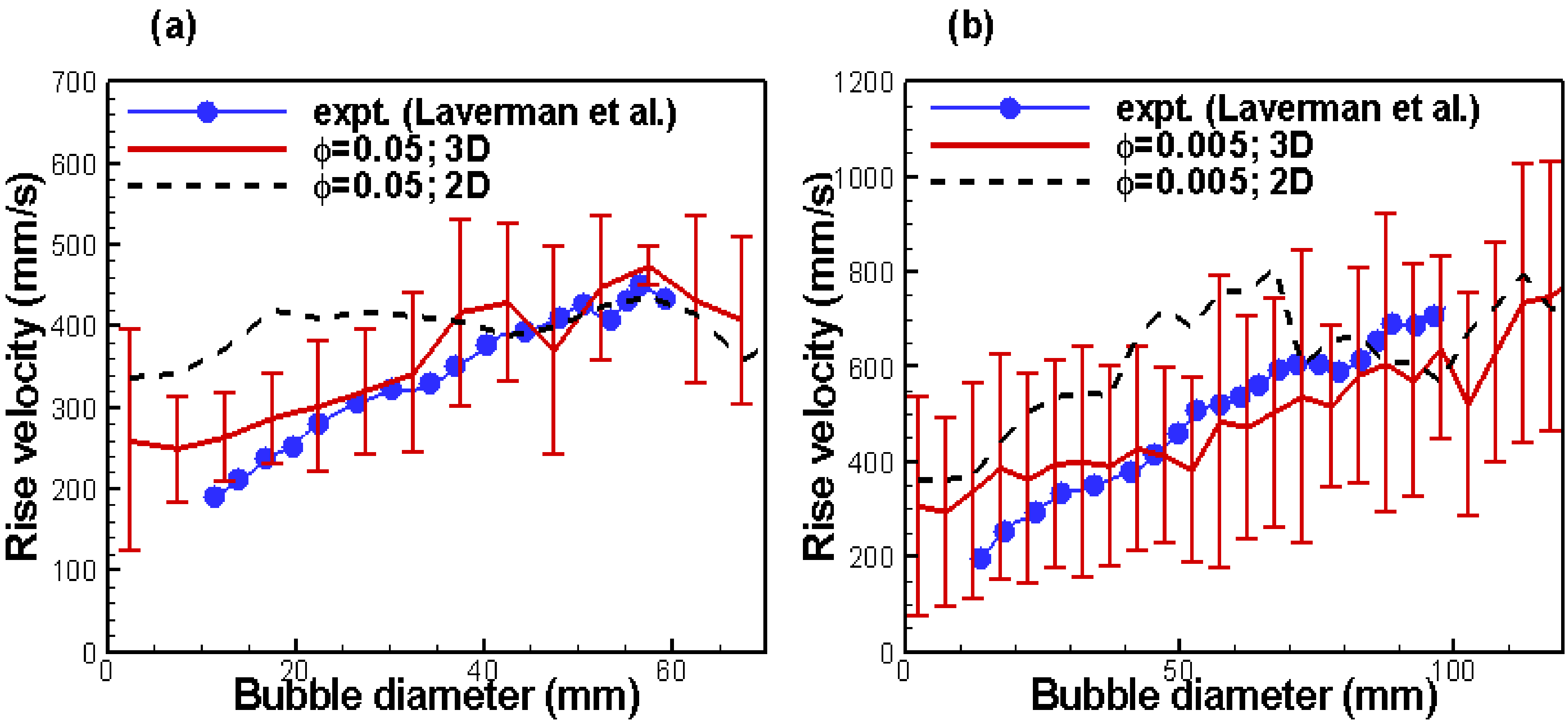


Predicted mean bubble diameters compared with experimental data for (a) $U_g = 1.5U_{mf}$; (b) $U_g = 2.5U_{mf}$ ($\varepsilon_{bndy} = 0.8$; $D_{b,min} = 5$ mm, diameter average).

Red: 3-D SImulations

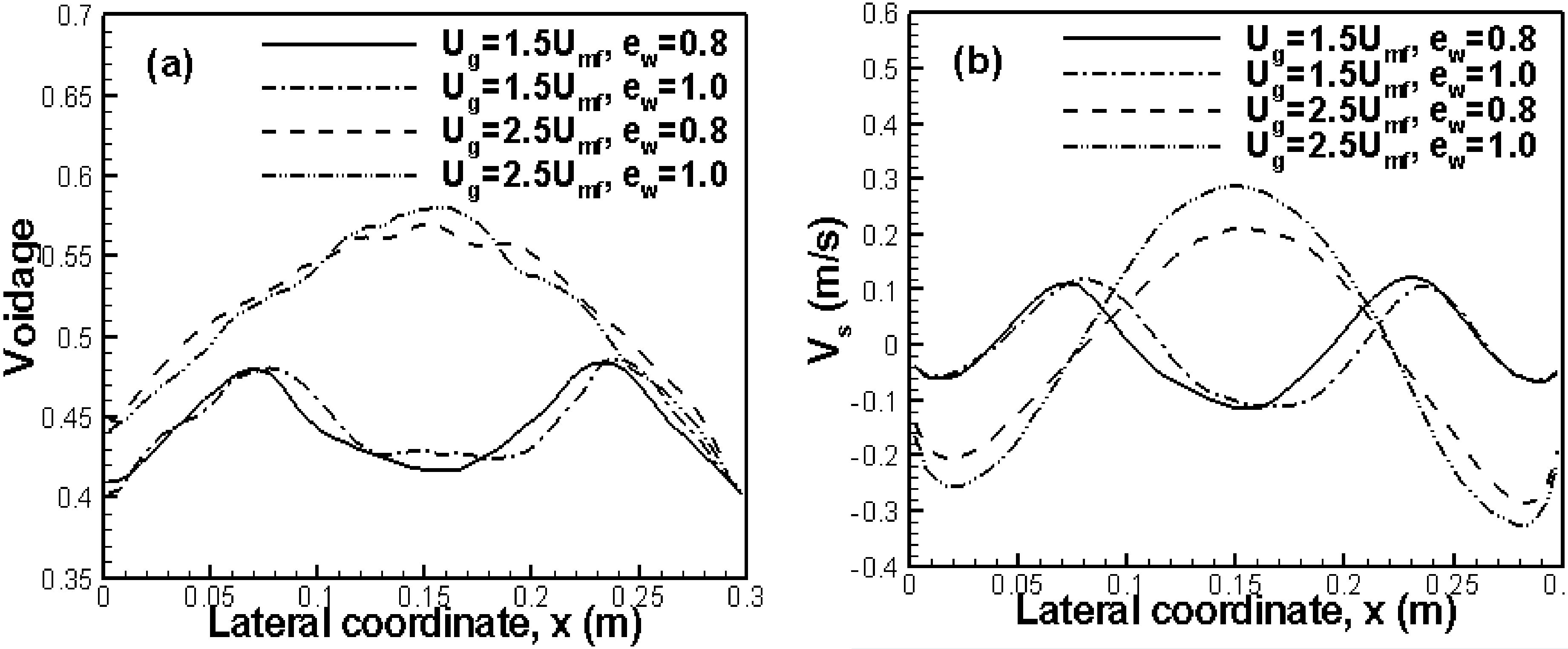
Blue: 2-D Simulations

Comparison with Experimental Bubble Rise Velocities



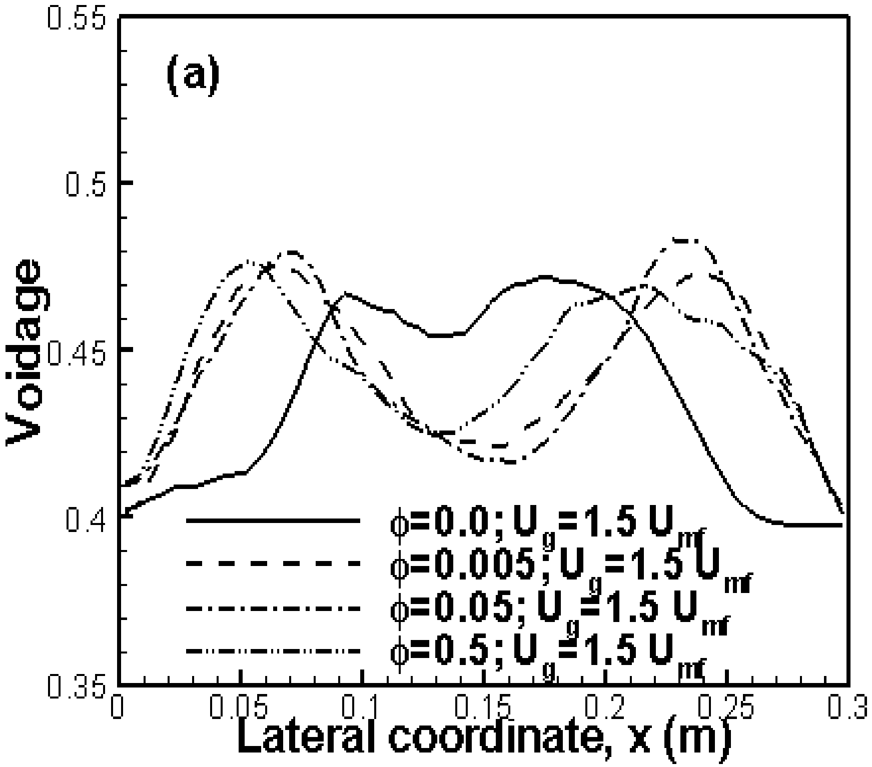
Average bubble rise velocity versus mean bubble diameters for (a) $U_g = 1.5U_{mf}$; (b) $U_g = U_{mf}$.

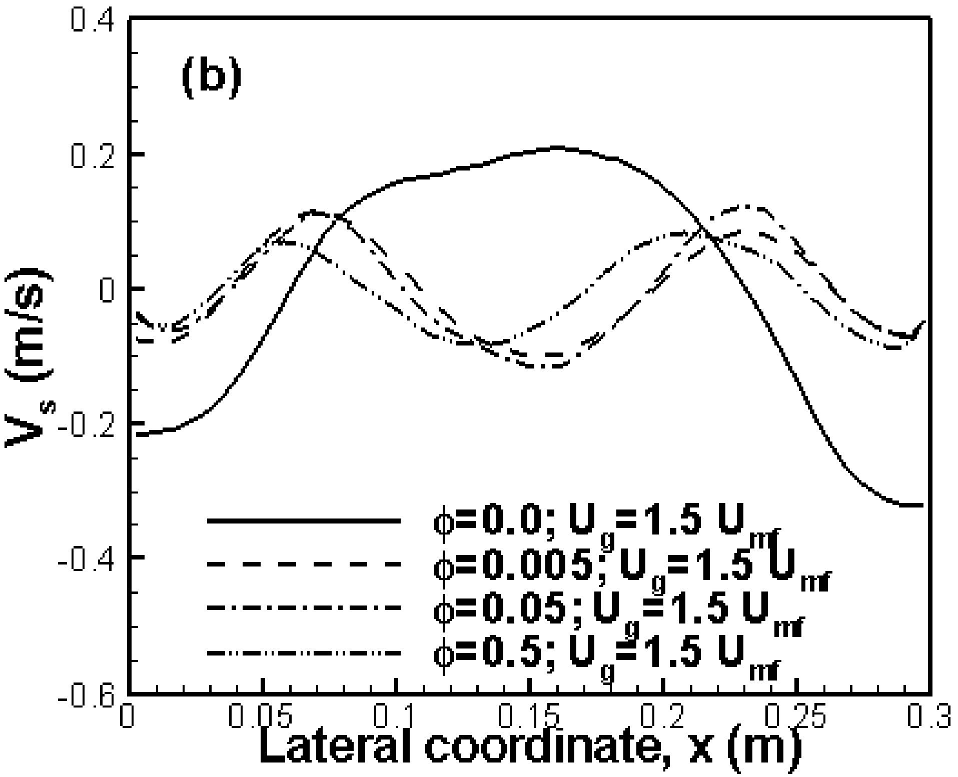
Effect of Particle/Wall Restitution Coefficient



Lateral profiles of time-mean (a) voidage, and (b) solid velocity at z = 0.2 m for different particle-wall restitution coefficients; 2-D simulations.

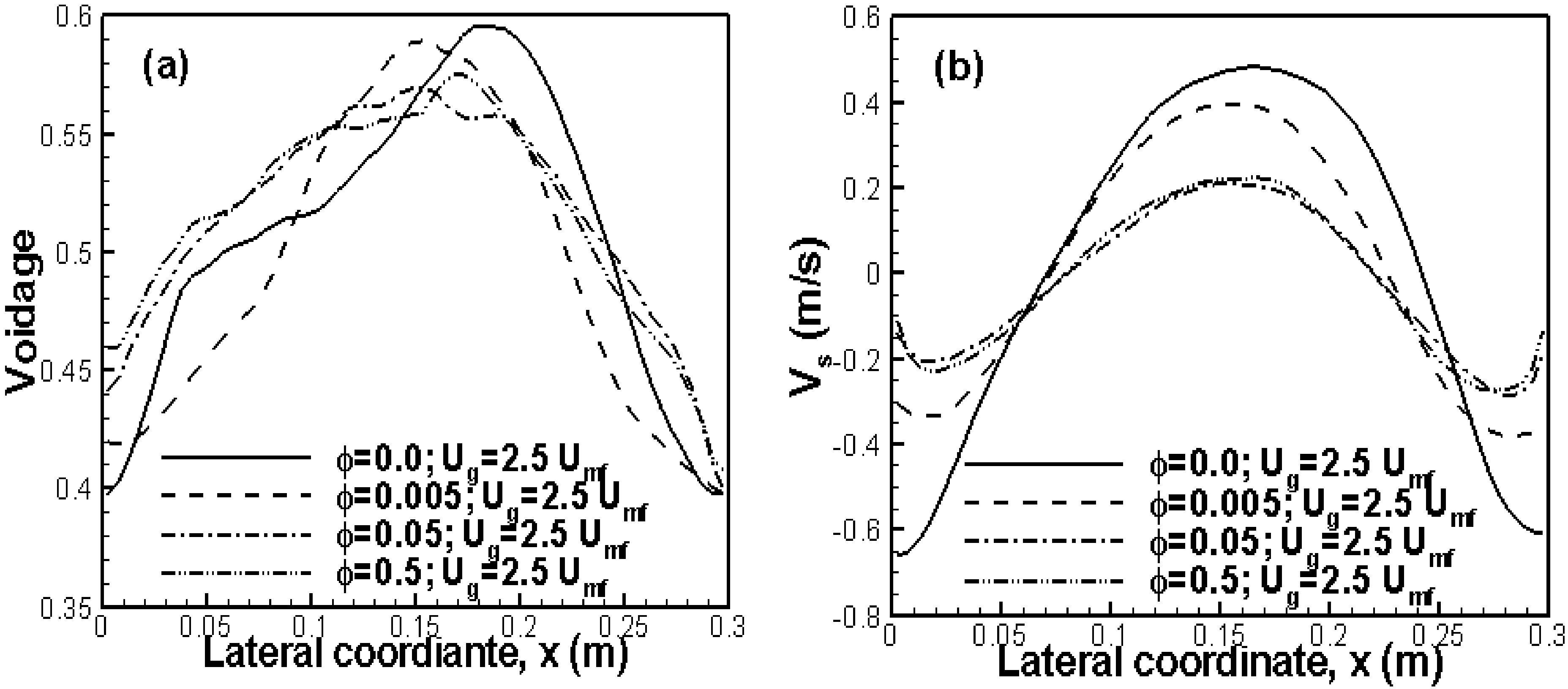
Effect of Wall Specularity Coefficient





Lateral profiles of time-mean (a) voidage, and (b) vertical solid velocity at z = 0.2 m for different specularity coefficients; 2-D simulations; U_g=1.5U_{mf}

Effect of Wall Specularity Coefficient



Lateral profiles of time-mean (a) voidage, and (b) vertical solid velocity at z = 0.2 m for different specularity coefficients by 2-D simulations; **U_g= 2.5U_{mf}**.

Summary: 2-D vs. 3-D Columns

- Wall boundary solid phase boundary condition again needs to be specified with great care.
- 3-D simulation of 2-D column is needed.
- Many factors, including bubble definition, minimum detectable bubble size, and averaging method, must be considered when comparing simulation predictions with experimental results.

3. Change in Volumetric Flow

- The volumetric flow of gas in fluidized beds reaction may vary with height due to
  - Chemical reactions: mole change:

    e.g. $CH_4 + 2H_2O \rightleftharpoons CO_2 + 4H_2$;
  - Decrease of flow due to gas addition or removal through jets or membranes;
  - Changes in temperature and/or pressure;
  - Change of phase: drying, condensation.

Numerical Model

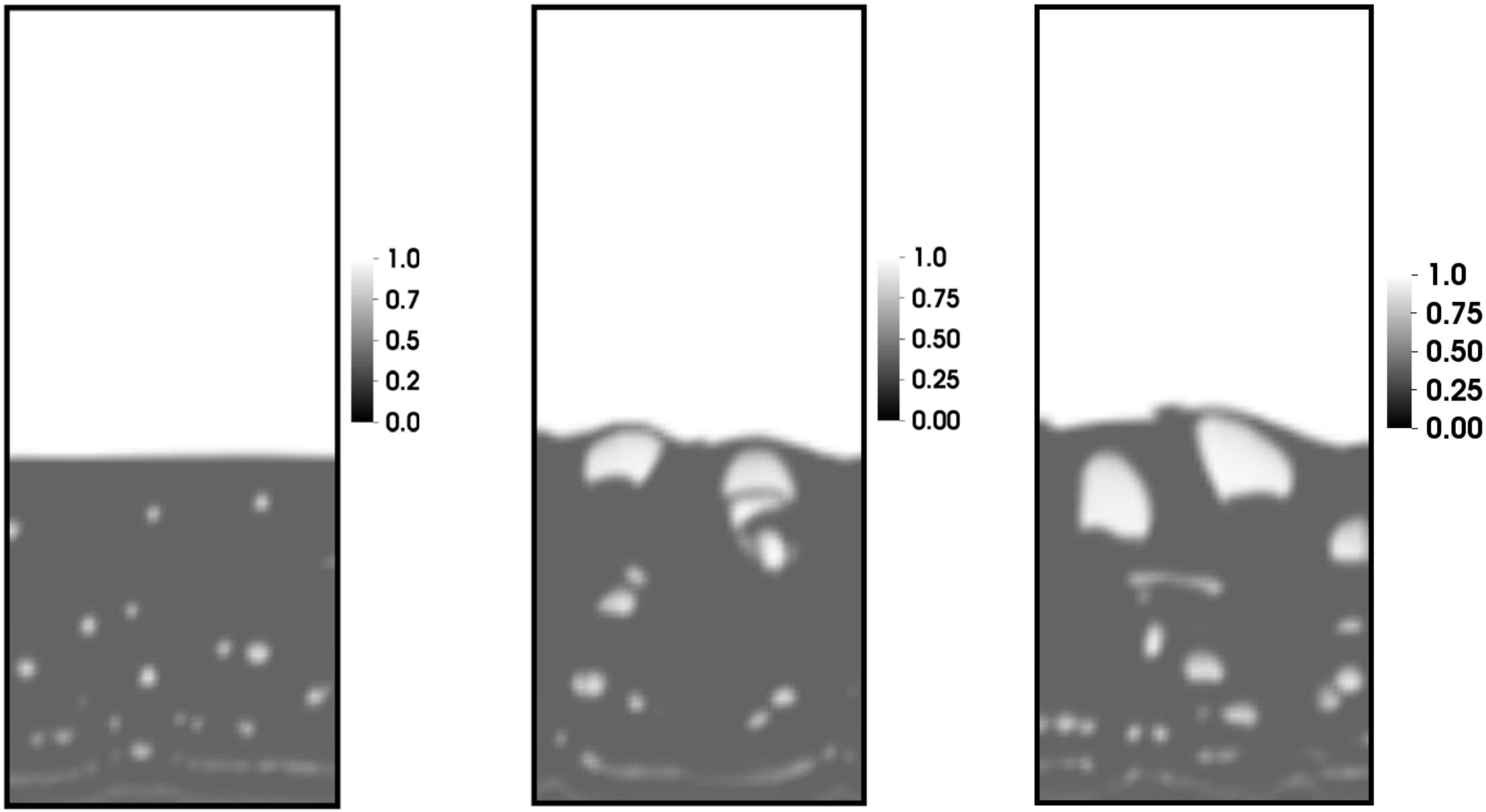
- 2-D simulation of change of volumetric flow in fluidized bed
  - Drying/condensation and Ozone decomposition reaction ($O_3 \rightarrow 1.5O_2$)
  - 485 µm glass beads, same Laverman et al. column (0.015 x 0.3 x 0.7 m)
- Numerical model
  - Eulerian-Eulerian model
  - MFIX

Drying and Condensation

- Simulation conditions

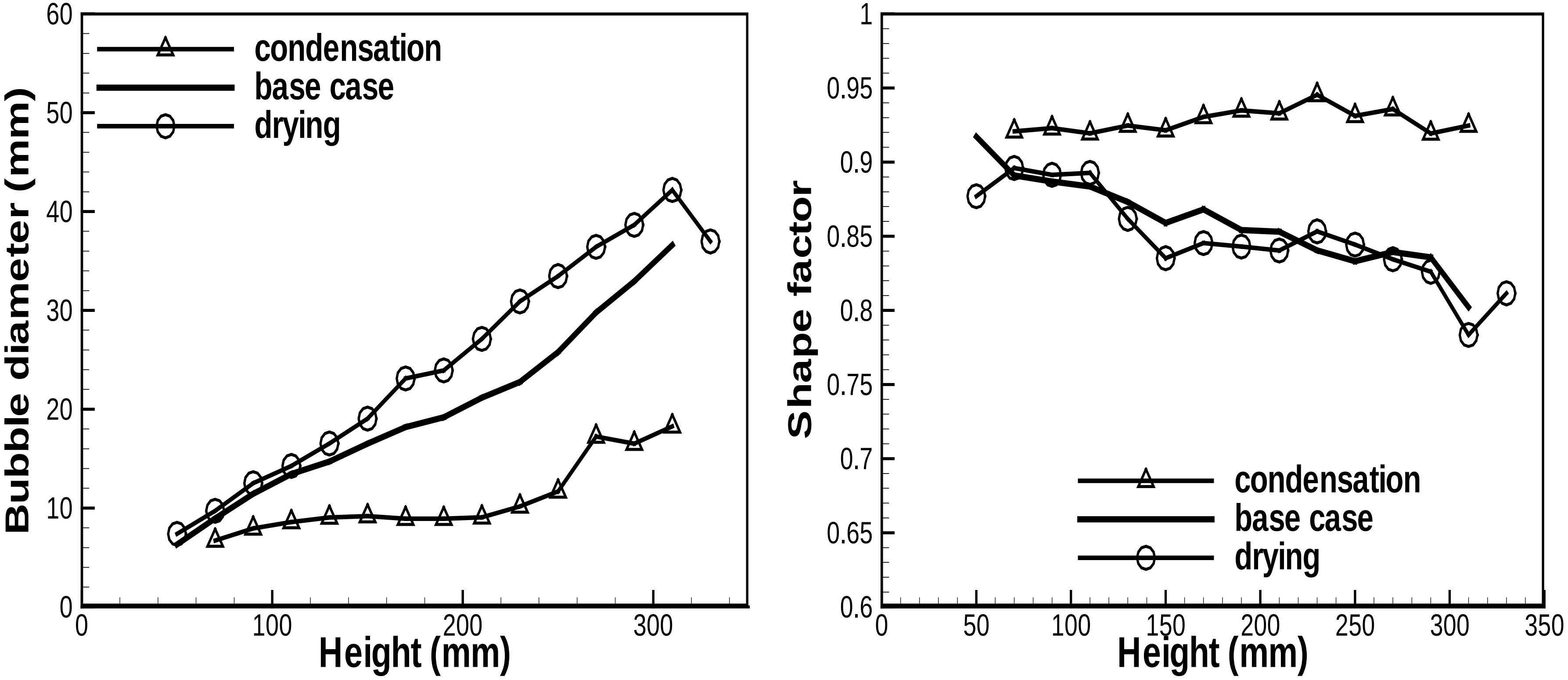
Parameters\Cases	**Condensation**	**Base Case**	**Drying**
U_g,bottom, m/s	0.24	0.24	0.24
U_g,exit, m/s	0.185	0.24	0.287
U_g,exit-U_{mf}, m/s	-0.009	0.046	0.093

Drying and Condensation



Snapshots of voidage contours for condensation (left), base case (middle), and drying (right).

Bubble Characteristics



Variation of average bubble diameter (left) and shape factor (right) with height for base case compared with cases with condensation and drying.

Chemical Reaction

Particle diameter = 0.50 mm

Parameters\Cases	**$3O_2$->$2O_3$**	**Base case**	**$2O_3$->$3O_2$**
U_g,bottom, m/s	0.24	0.24	0.24
U_g,exit, m/s	0.208	0.24	0.277
U_g,exit-U_{mf}, m/s	0.014	0.046	0.083

Particle diameter = 0.20 mm

Parameters\Cases	**$3O_2$->$2O_3$**	**Base case**	**$2O_3$->$3O_2$**
U_g,bottom, m/s	0.09	0.09	0.09
U_g,exit, m/s	0.077	0.09	0.112
U_g,exit-U_{mf}, m/s	0.039	0.052	0.074

Summary: Effect of Volume Change

- For coarse particles, bubble size is predicted to increase or decrease significantly due to volumetric flow changes in the dense phase.
- For fine particles, changes in bubbles size are predicted to be small for volumetric flow changes in the dense phase.
- Defluidization might occur for decreases in volumetric flow, but this needs further study.
- Experimental work is in progress on effect of step changes (up and down) in pressure.

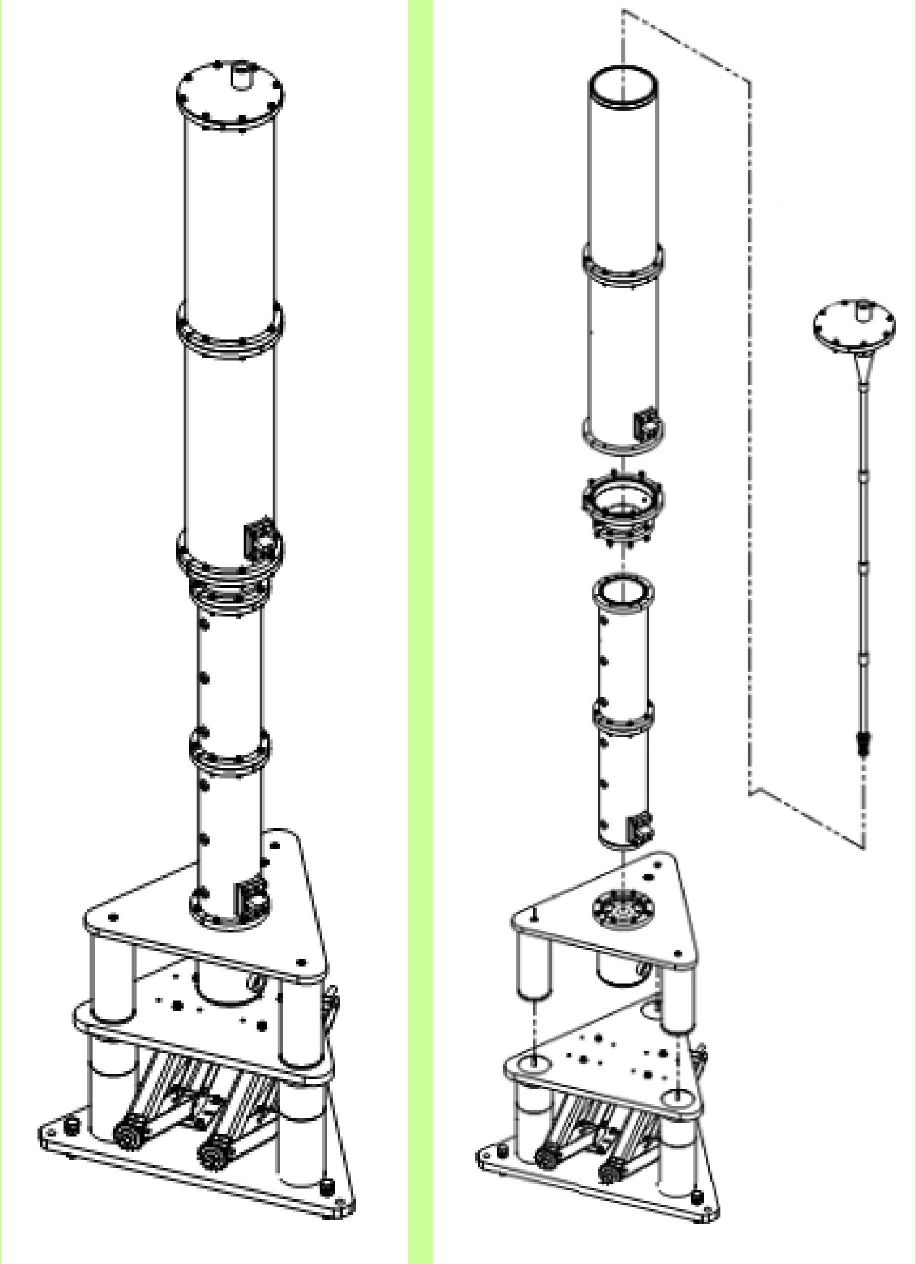
4. Particle Velocity/Travelling Fluidized Bed

Column designed & constructed to travel from location to location. Co-application by a team of researchers from five Canadian universities (UBC, Calgary, Saskatchewan, Western Ontario, Ecole Polytechnique) funded by NSERC.

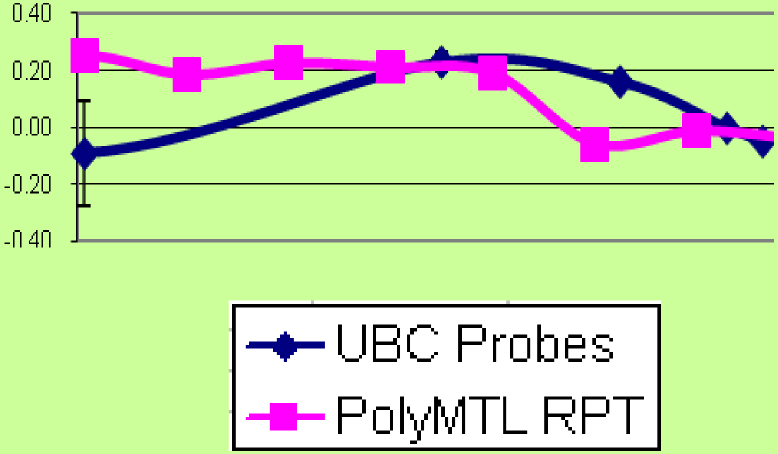
Objectives: **1**. Compare and evaluate advanced experimental methods of measurement.

2. Provide a unique comprehensive database for validation of CFD codes.

3. Provide a method for evaluating probes that can be deployed in industrial units.



Traveling fluidized bed (TFB) column:
a) assembled, b) exploded modular view



Example of difference in measured mean particle velocities.

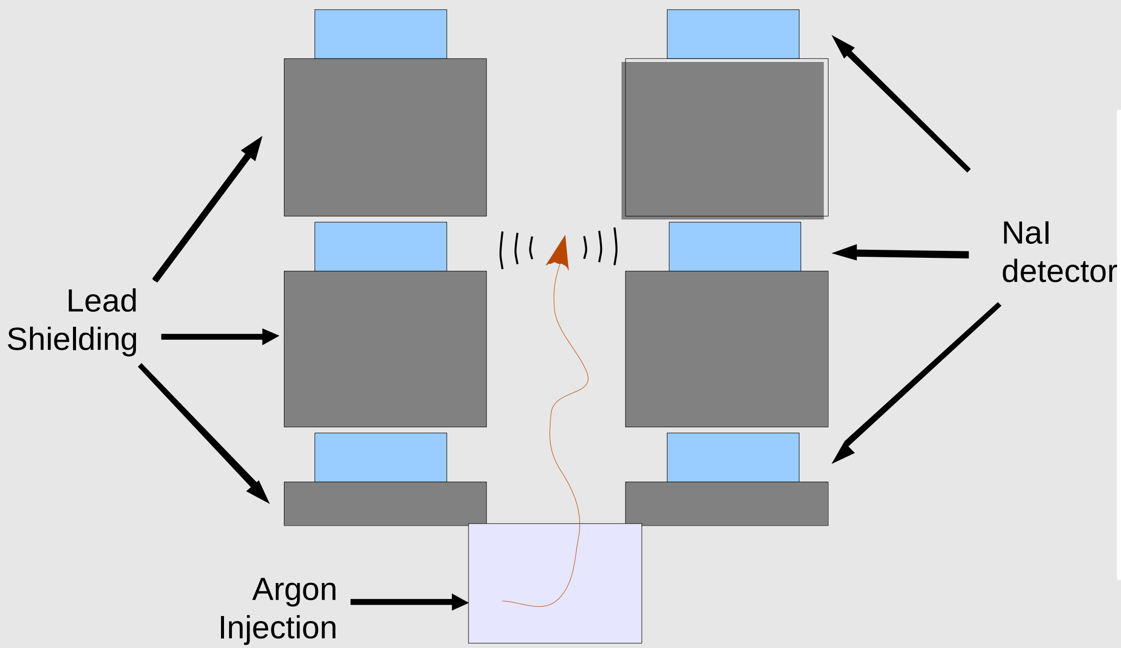
One Dilemma

- Reasonably good agreement with respect to voidage measurements from different techniques
- However, significant differences between particle velocity measurements for:

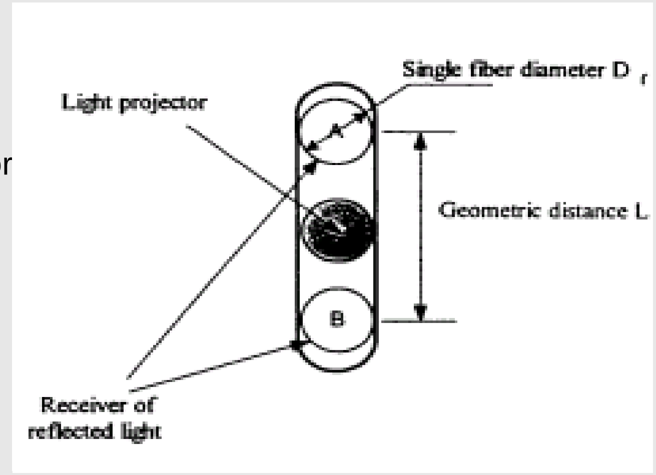
➢ **Radioactive particle tracking**: (Chaouki et al.) follow a single particle trajectory over a very long time period.

➢ **Optical probes**: cross-correlate signal from particles passing vertically aligned fibres.

Can CFD help sort out whether the differences are reasonable?



RPT experiment schematic



Optical fibre probe

Other Areas for Complementary Work

- Effect of electrostatics on hydrodynamics and entrainment;
- Non-uniformity of multiphase flow through identical parallel paths;
- Determining bubble properties from pressure fluctuations;
- Distributor: influence of the windbox on hydrodynamics;
- Fluidization of particles of extreme shapes, e.g. biomass particles;
- Dynamics of liquid-fluidization inversion;
- Jets entering fluidized beds;
- Fluidization around baffles, e.g. sheds.

Acknowledgement

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