Evaluation of Drag Models for Gas-Solid Fluidization of Geldart A Particles in All Flow Regimes

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Presentation Outline

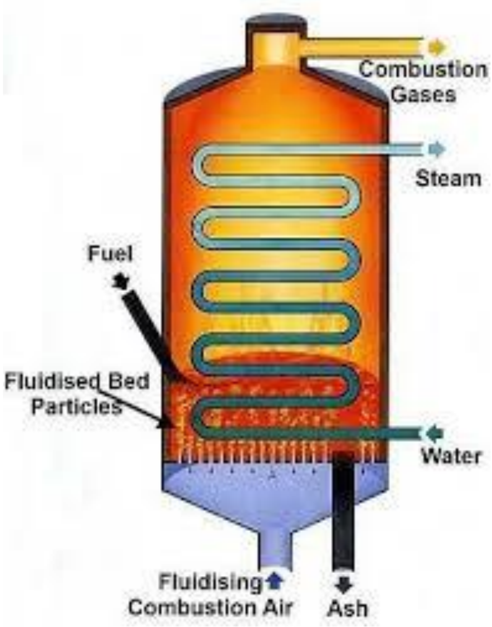
- Motivation
- Multiphase CFD and coarse grid simulation
- Development of sub-grid drag closure
- Validation of drag model in all fluidization regimes
- Summary of results

Applications of Fluidized Beds

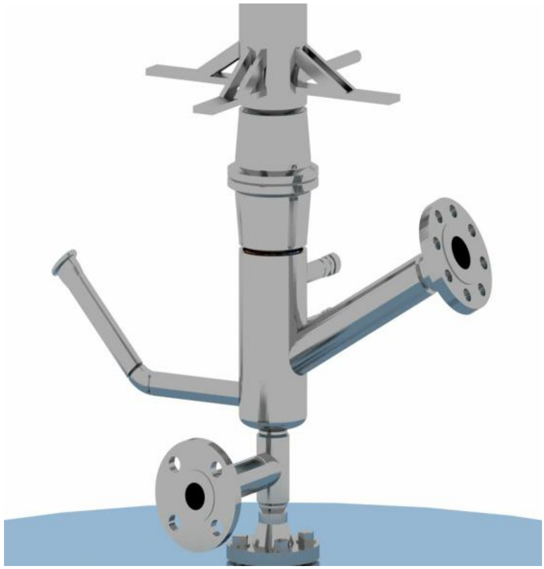
- Fluidized bed has attracted attention for several decades and has been widely used in chemical, petrochemical, and energy industries.
- Such as FCC processes, polymerization processes, MTO processes, combustion processes, **biomass thermal conversion**, **biomass vapor phase upgrading (VPU) process**.
- Advantages: high-throughput capabilities, excellent heat and mass transfer characteristics, and superior reaction rates of gas-solid mixtures.

FCC process

MTO process



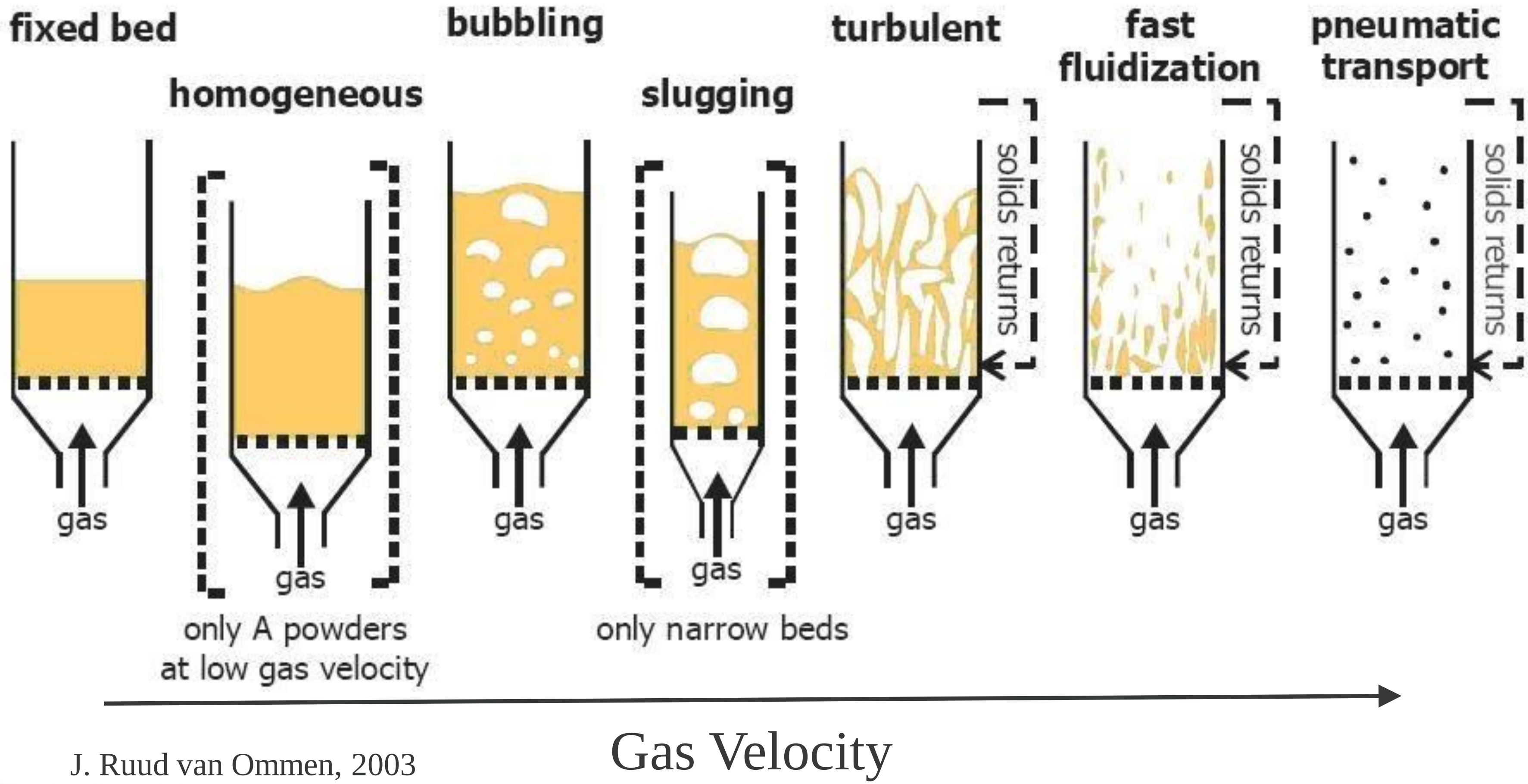
Combustion process



Biomass VPU process

Gas-Solid Fluidization Regimes

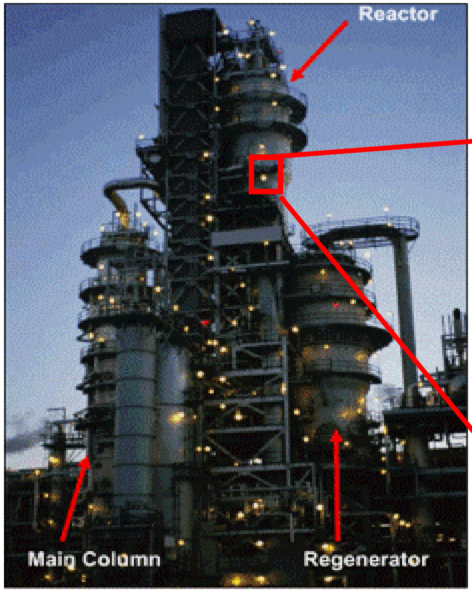
- Fluidized bed: A typical fluidized bed is a cylindrical column in which solid particles are suspended in a fluid at a certain fluid velocity.
- Increasing of gas velocity, several fluidization regimes can be observed.
- Gas-solid fluidization is very complex.

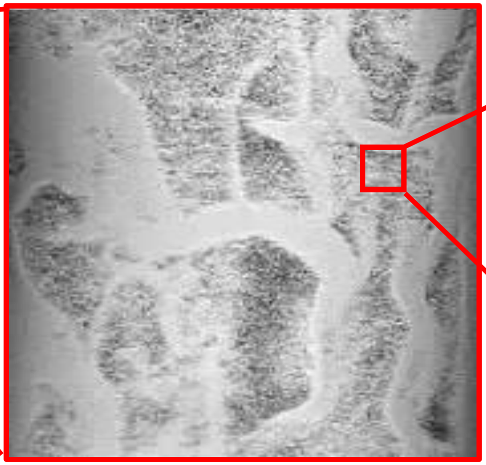


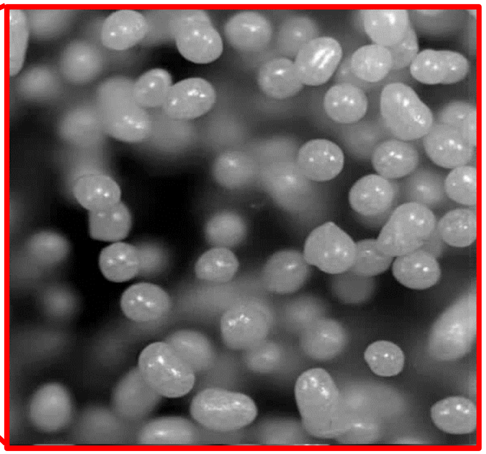
J. Ruud van Ommen, 2003

Multi-Scale Structure of Gas-Particle Flows

- From macroscale to microscale







Macroscale

- Large length and time scale
- Large number of particles

Mesoscale

- Particle segregation
- Clustering or bubbling
- Turbulence modulation

Microscale

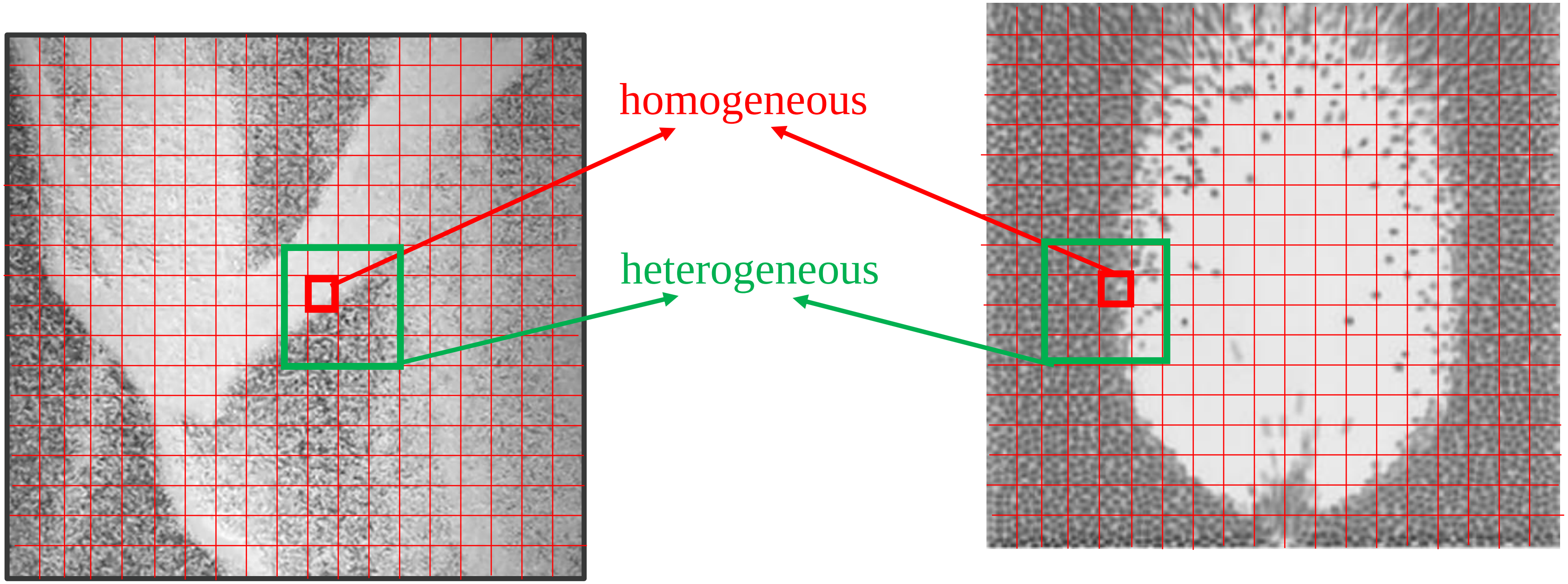
- Particle interactions
- Particle shape
- Phase change
- Wakes

Pictures credits: Frank Shaffer et al., *Powder Technology*, 2013, 86-99

Why Coarse-Grid Simulation?

- Drag models for gas-solid flow simulation
  - "Standard" drag models are based on homogeneous solids distribution assumption
  - They work best for fine grid simulations where solids are more homogeneous
  - Coarse-grid simulations tend to over-predict the drag force.

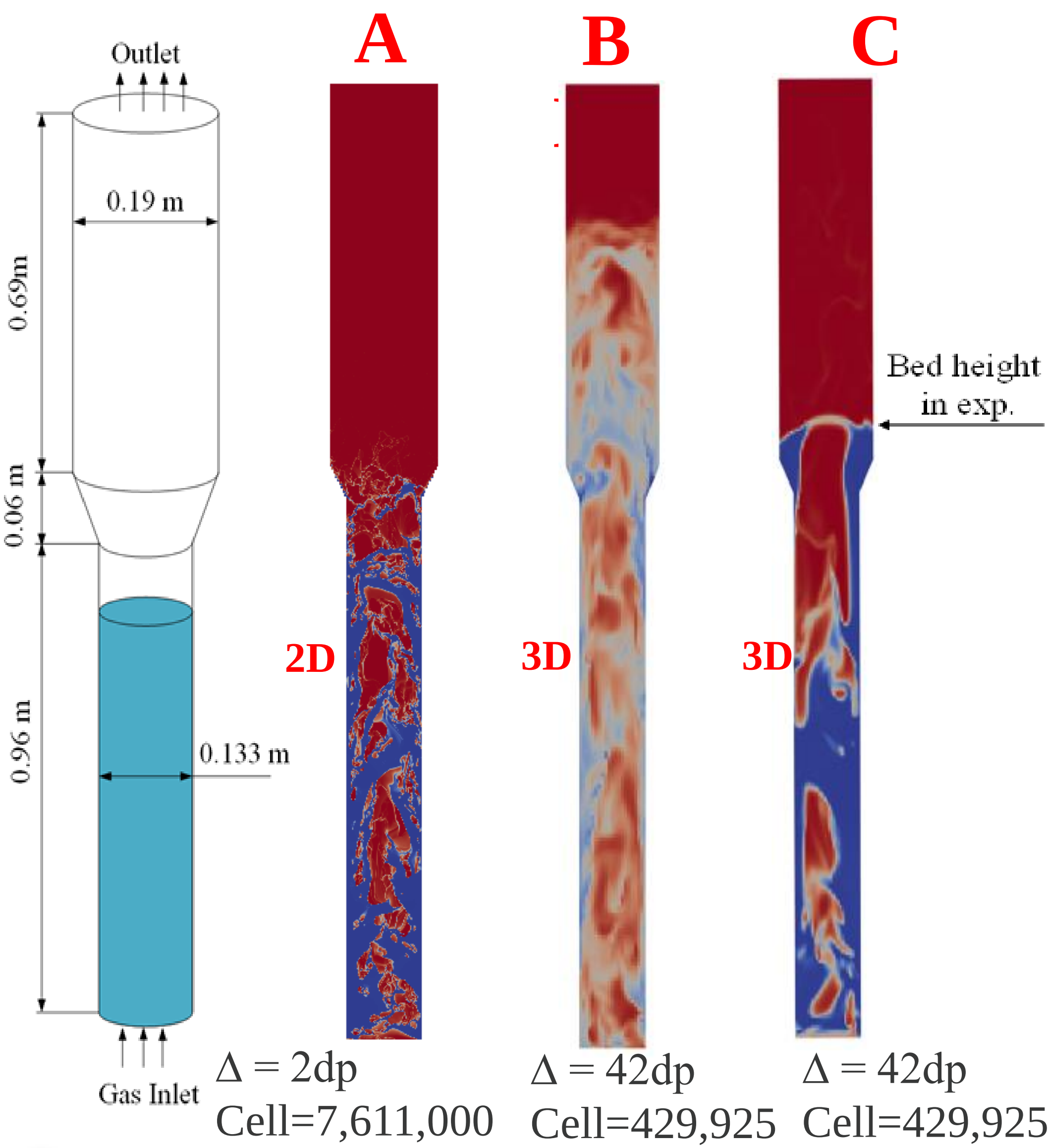
- Fine-grid simulation is very expensive, especially for
  - Small particles belong to Geldart A (dp=~100 microns)
  - Grid-independent requires computational grid Δ=~ 2-10 dp
  - Fine grid simulation of industrial-scale reactors is impractical, such as FCC unit, 2D, $O(10^6)$; 3D, $O(10^9)$.
  - Coarse grid simulation with Δ=~100-1000dp is required for industrial-scale reactor simulations.



Fine grid Risers: Δ=~ 10 dp

Fine grid Bubbling: Δ= ~ 2-4 dp

Coarse-Grid Simulations Need Sub-Grid Closures



A-fine grid with standard drag model
B-coarse grid with standard drag model
C-target result with proper coarse-grid model

- Coarse grid simulation needs to account for sub-grid effect.
- Sub-grid gas-solid drag model is the most critical part.
- The homogeneous drag model has the form

$$F_d = \beta(ug - us)$$

- The heterogeneous drag model introduces a correction factor, C

$$F_d = \beta(u_g - us)\boldsymbol{H}$$

How To Obtain Heterogeneous Drag Models?

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- **Homogeneous drag model (Applicable to highly resolved simulations of small scale systems)**
  - Derived from experiment or correlations: Wen and Yu, 1996; Ergun, 1952; Gidaspow, 1994
  - Derived from PR-DNS of randomly arranged particles: BVK (Beetstra et al., 2005); HKL (Hill et al., 2001); TGS (Tenneti et al., 2011)
- **Heterogeneous drag model-- considering mesoscale structure (Applicable to coarse-grid simulations of large scale systems, used for scale-up)**
  - Derived from mesoscale structure method: EMMS (Li and Kwauk, 1994)
  - ✓ Derived from fine grid two-fluid model: Igci et al., 2008; Sarkar et al., 2016
  - Derived from fine grid CFD-DEM model: Radl and Sundaresan, 2014
  - Derived from PR-DNS of cluster configurations: MMS (Mehrabadi et al., 2016)

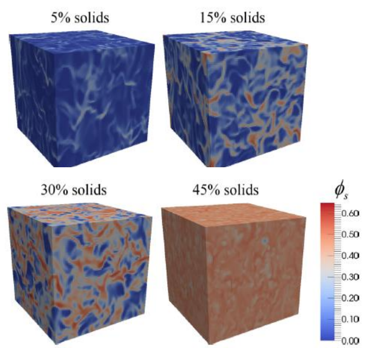
Heterogeneous Drag Derived From Fine Grid Two-Fluid Simulation

- Homogeneous drag model

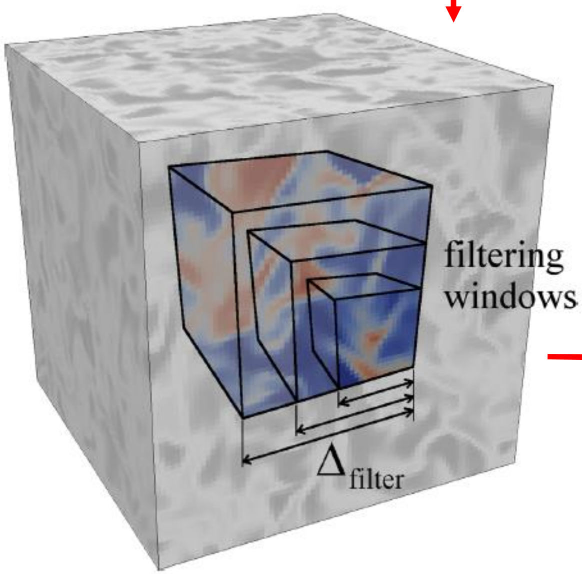
$$\beta_{Wen-Yu} = \frac{3}{4}\frac{\alpha_g(1-\alpha_g)\rho_g|\overrightarrow{u_g}-\overrightarrow{u_s}|}{d_s}C_{D0}\alpha_g^{-2.65}$$

- Heterogeneous drag model

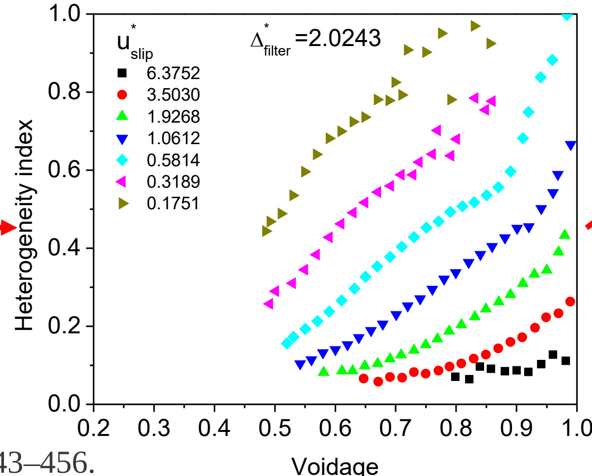
$$\beta_{Sarkar} = \beta_{Wen-Yu}H$$



Fine grid simulation

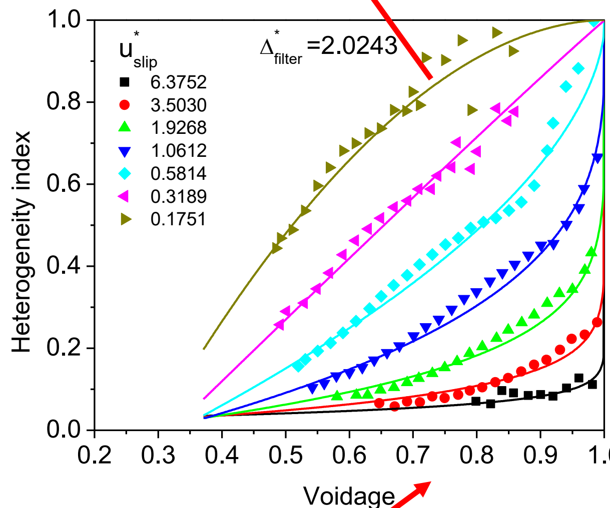


Filtering



Fitting

(Voidage, slip velocity, filter size)



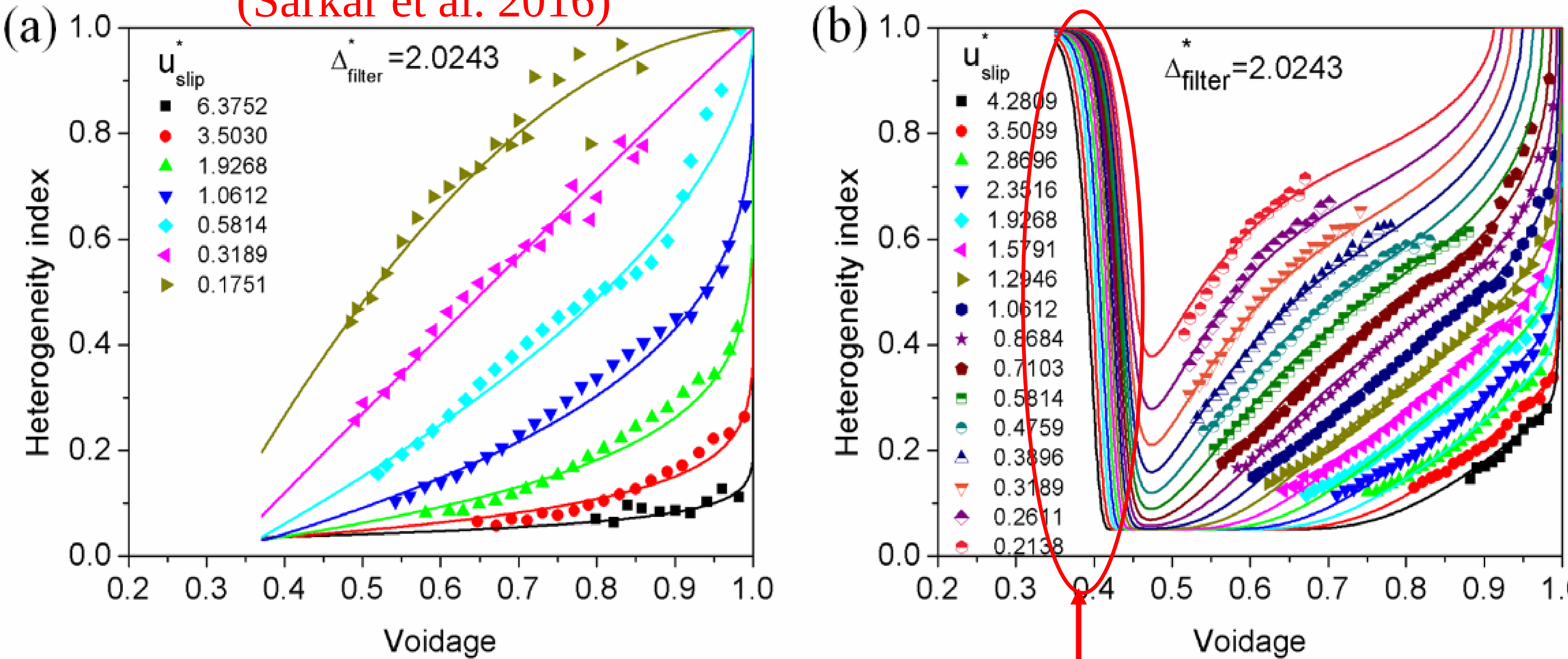
Sarkar et al., 2016, Chemical Engineering Science,152, 443–456.

New Filtered Drag Model

- In theory, the heterogeneity index should approach 1 near the maximum solids-packing limit, the flow becomes homogeneous and no sub-grid corrections are needed.
- A new drag model was developed.
- A more realistic limit was imposed at the dense regime.

Original Sarkar filtered drag model (Sarkar et al. 2016)

New filtered drag model



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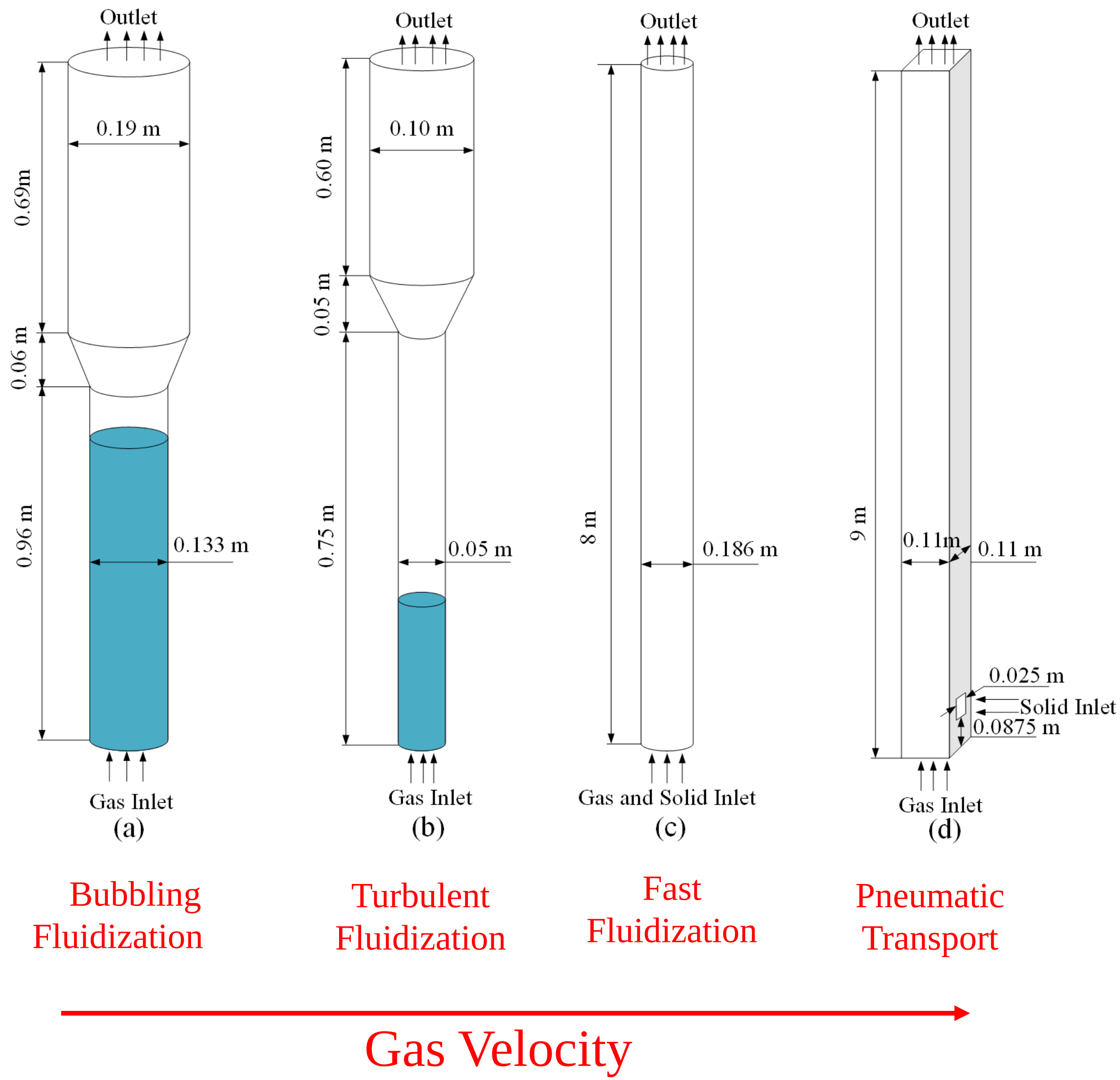
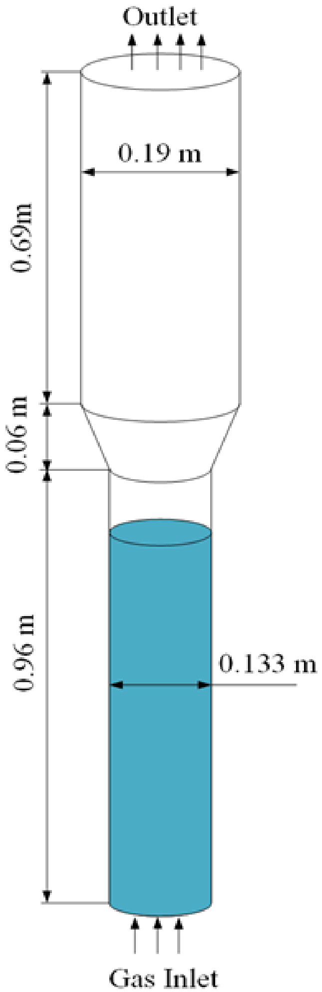
Determine the Optimal Drag Model for Fluidization Simulation

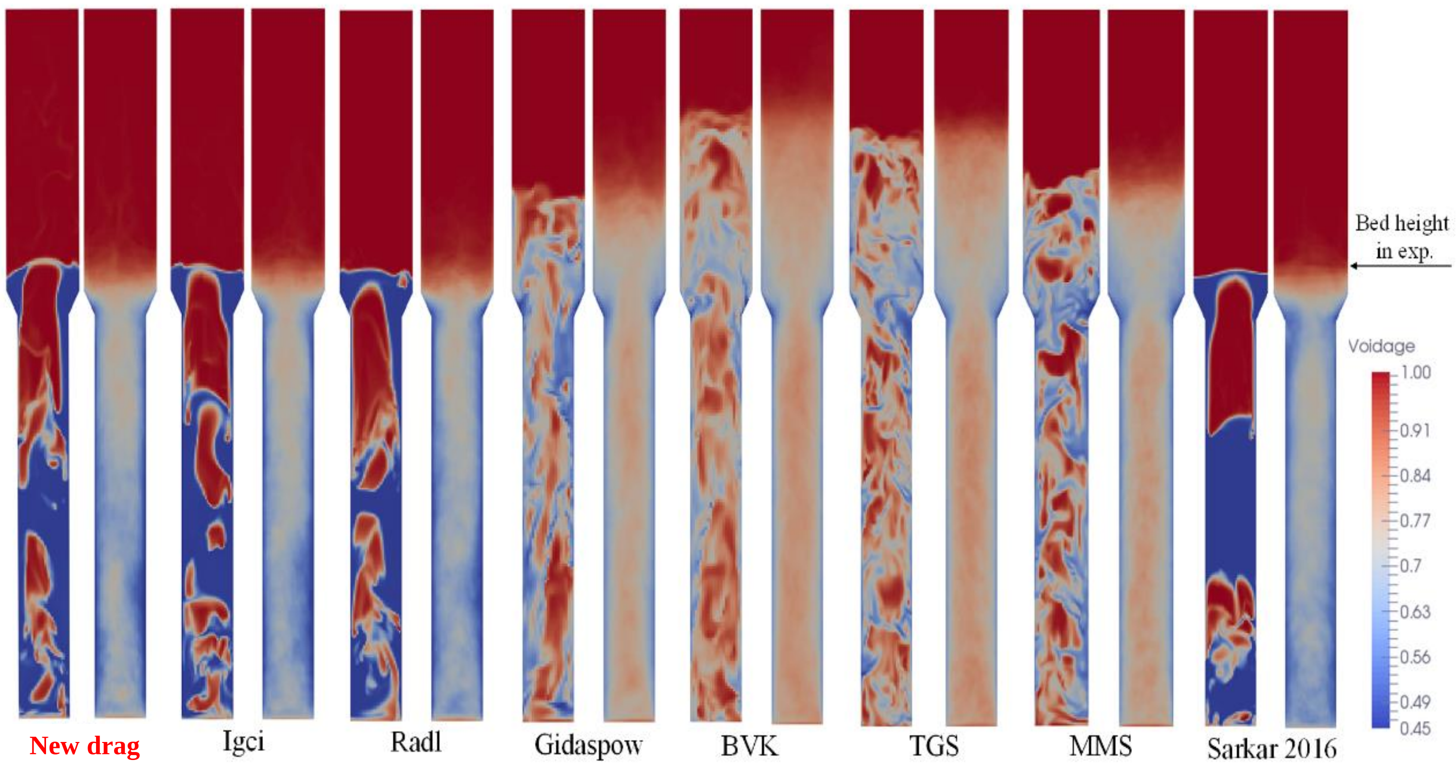
- A comprehensive evaluation of drag models for **Group A** particles was performed
  - **Eight drag** models were evaluated
  - Detailed, **three-dimensional** simulations were conducted
  - **A range of fluidization regimes** were modeled
  - Model results were compared to **experimental data** from the literature



Determine Best Drag Model for Bubbling Fluidization

- The "Traveling fluidized bed" by Dubrawski et al. (2013)

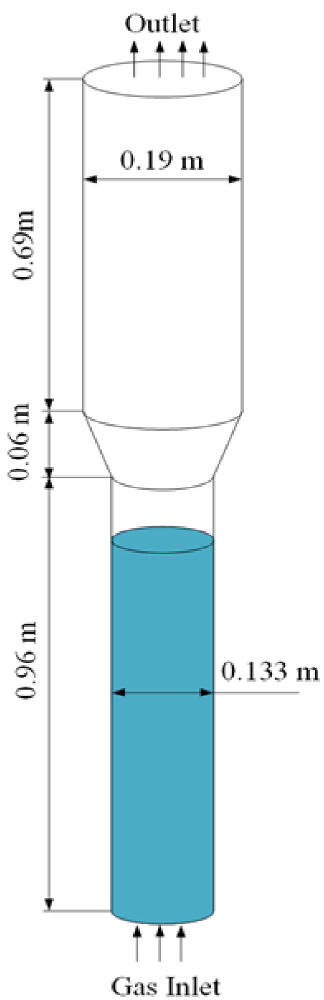


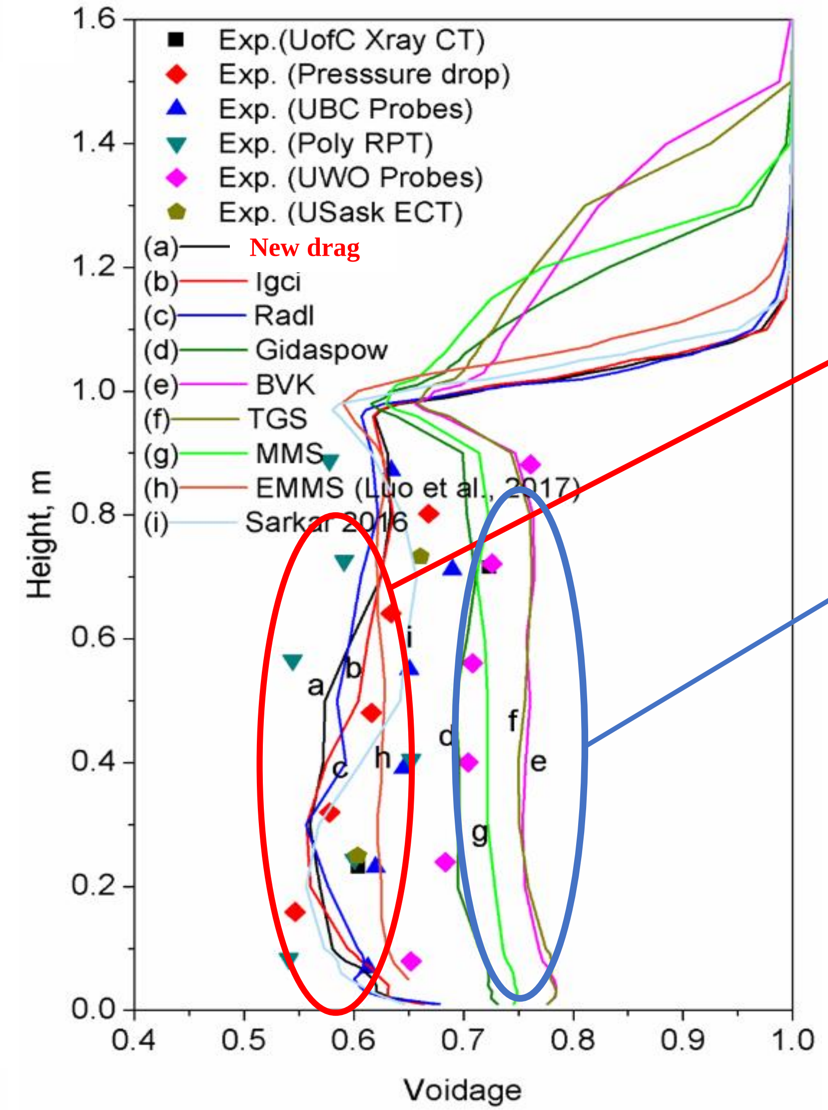


Figures show the instantaneous and time averaged bed voidage using different drag models

Determine Best Drag Model for Bubbling Fluidization

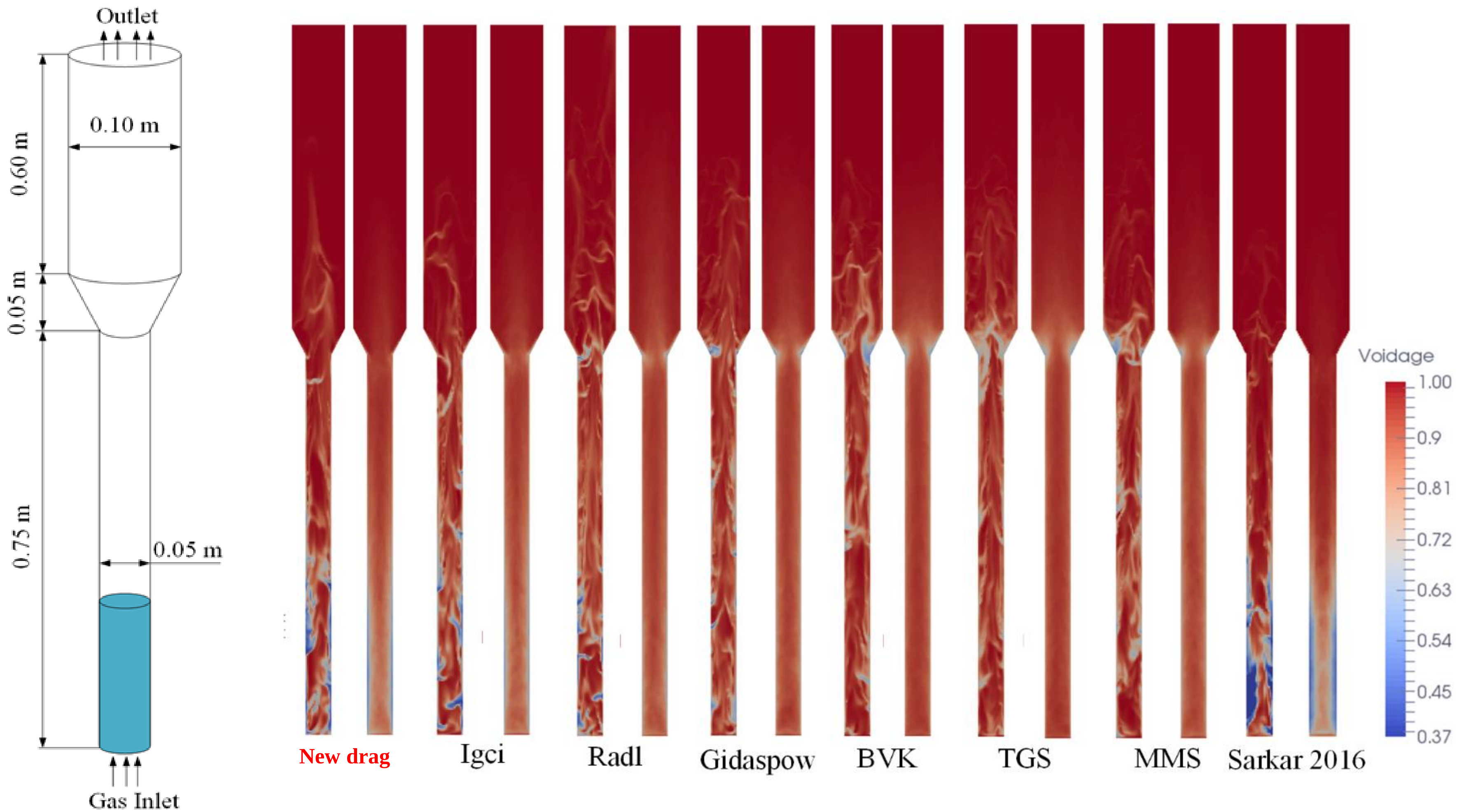
- Compare the axial profile of time-averaged voidage





- Note the variation in experimental measurements
  - Pressure drop (◆) is a standard technique
- Best agreement with heterogeneous drag models (New drag, Igci, Radl, EMMS)
- Homogeneous drag models over predict the bed voidage
- Ref: Dubrawski et al. (2013)

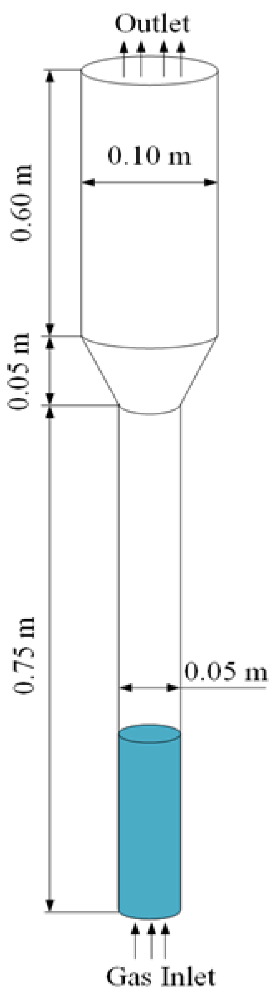
Determine Best Drag Model for Turbulent Fluidization

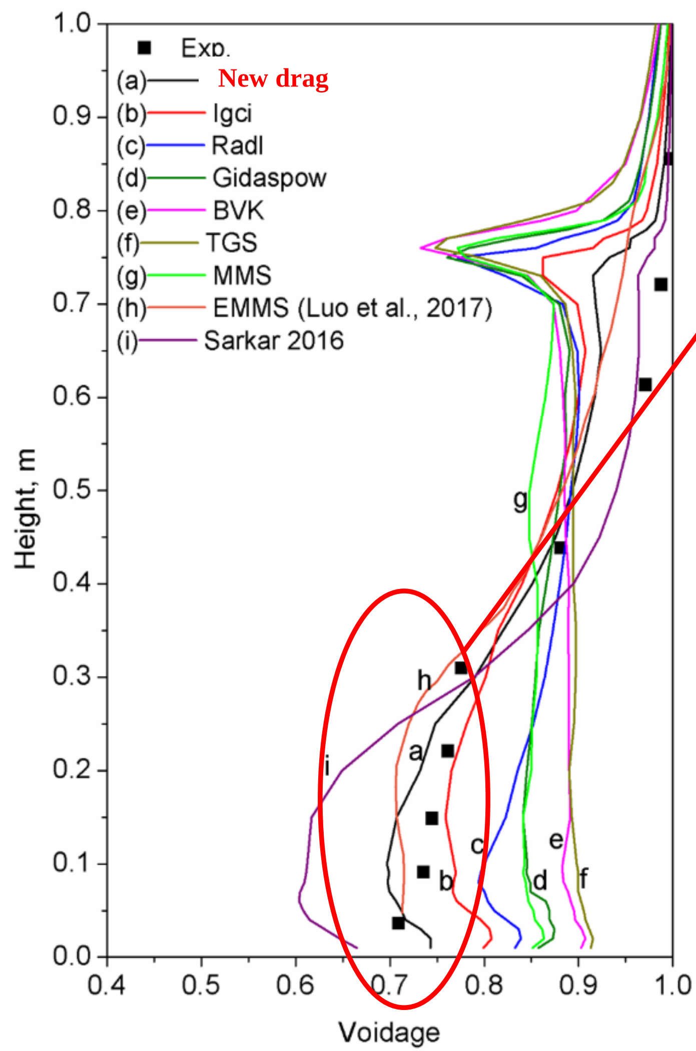


Figures show the instantaneous and time averaged bed voidage using different drag models

Determine Best Drag Model for Turbulent Fluidization

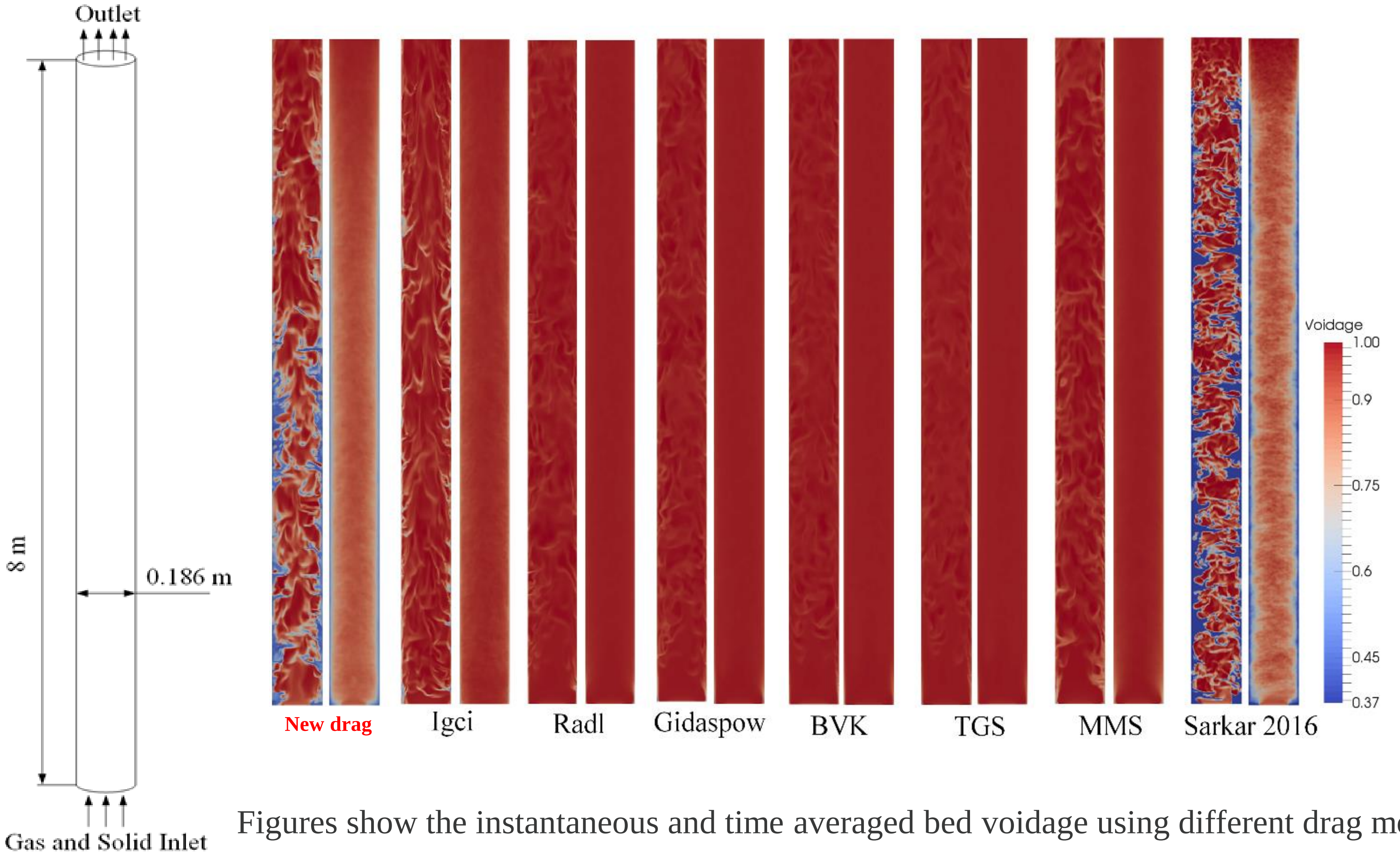
- Compare the axial profile of time-averaged voidage





- The experimental measurement are pressure drop values
- Best agreement with heterogeneous drag models
  - (a) New drag
  - (b) Igci et al.
  - (h) EMMS (from literature)
- The Sarkar 2016 drag model underpredicted the voidage in the bottom regime.
- Ref: Venderbosch (1998)

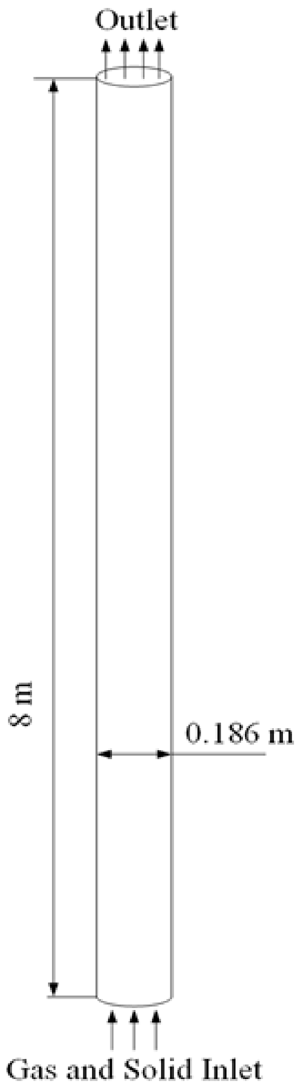
Determine Best Drag Model for Fast Fluidization

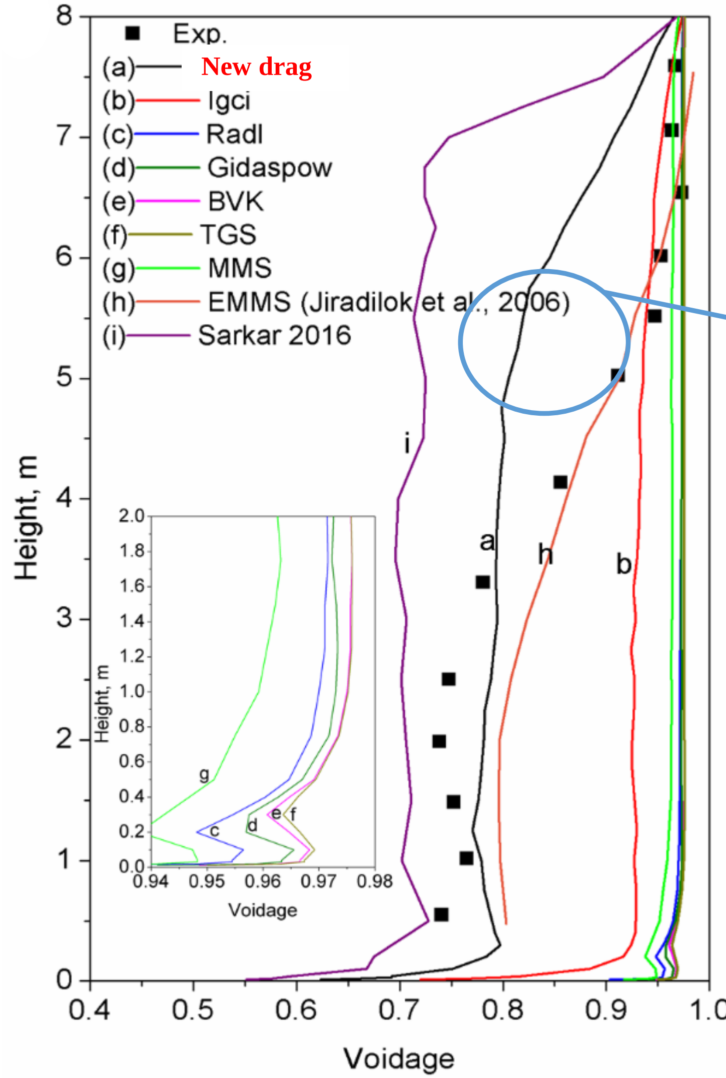


Figures show the instantaneous and time averaged bed voidage using different drag models

Determine Best Drag Model for Fast Fluidization

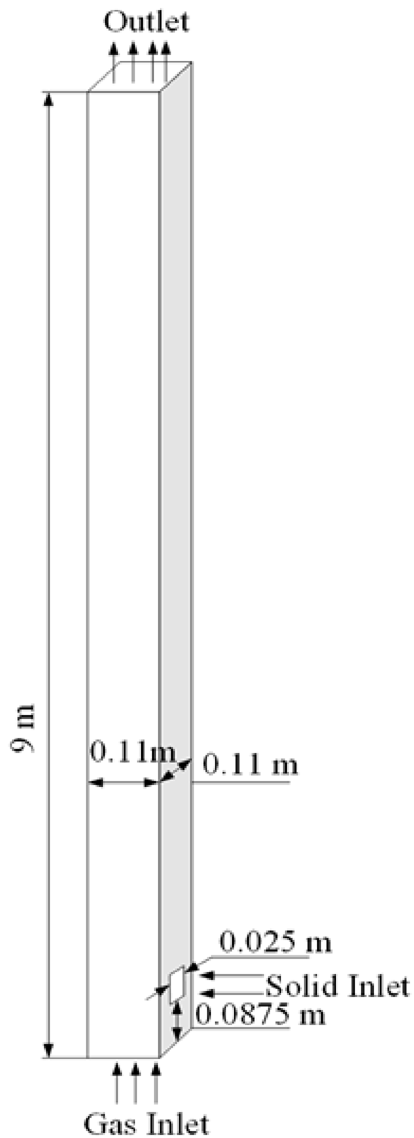
- Compare axial profile of time-averaged voidage

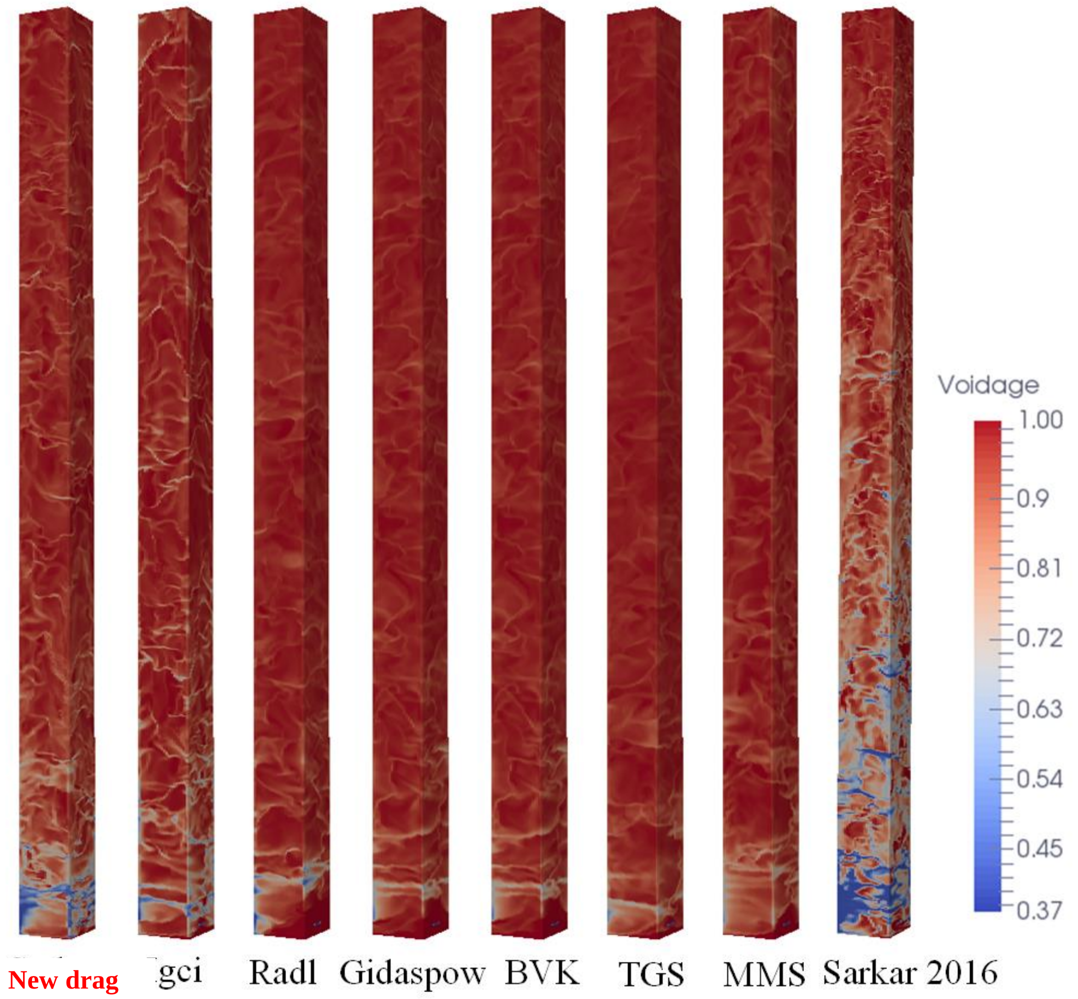




- Experimental measurement: Fiber optic probe
- Best agreement with heterogeneous drag models
  - (a) New drag *(note the under-prediction in the upper region)*
  - (h) EMMS *(from literature)*
- The Sarkar (2016) drag model without a dense limit correction significantly under predicted the voidage in the fast fluidized.
- Ref: Wei et al. (1988)

Determine Best Drag Model for Pneumatic Transport

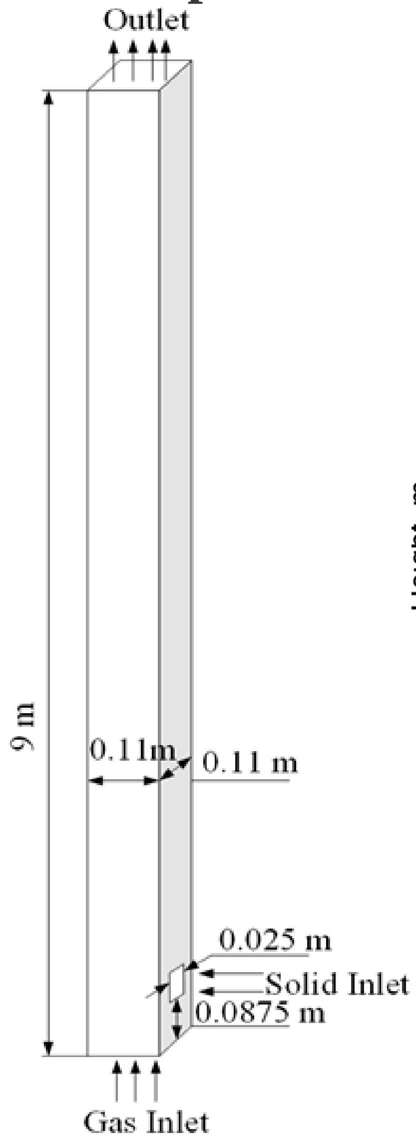


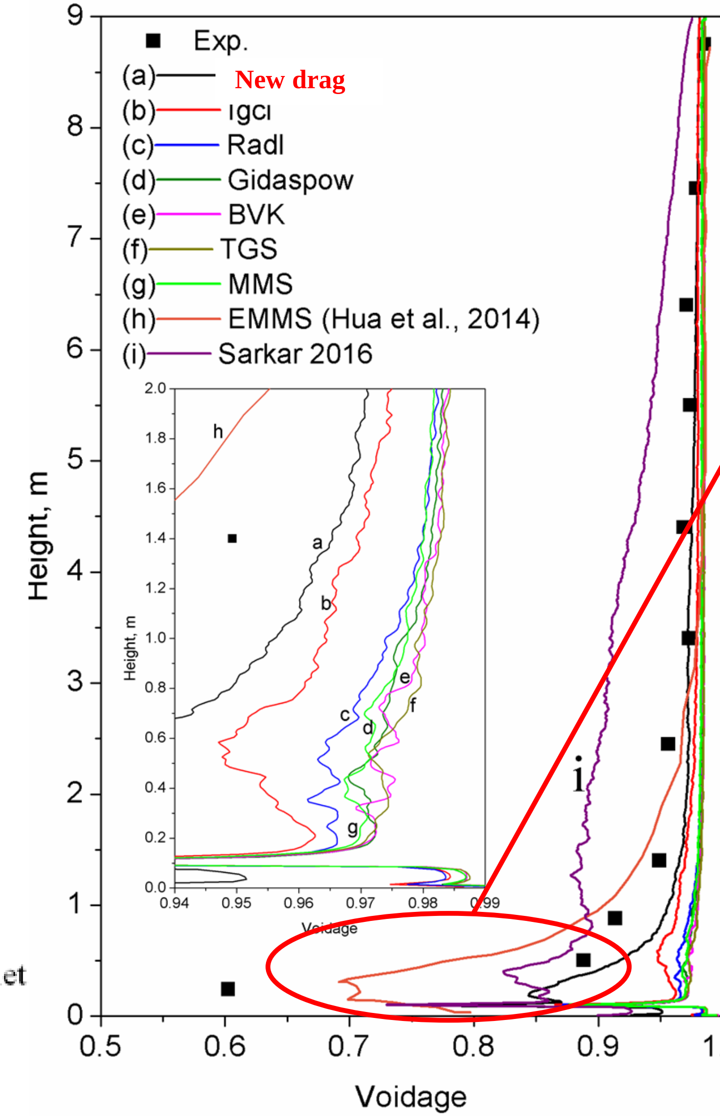


Figures show the instantaneous bed voidage using different drag models

Determine Best Drag Model for Pneumatic Transport

- **Compare axial profile of time-averaged voidage**





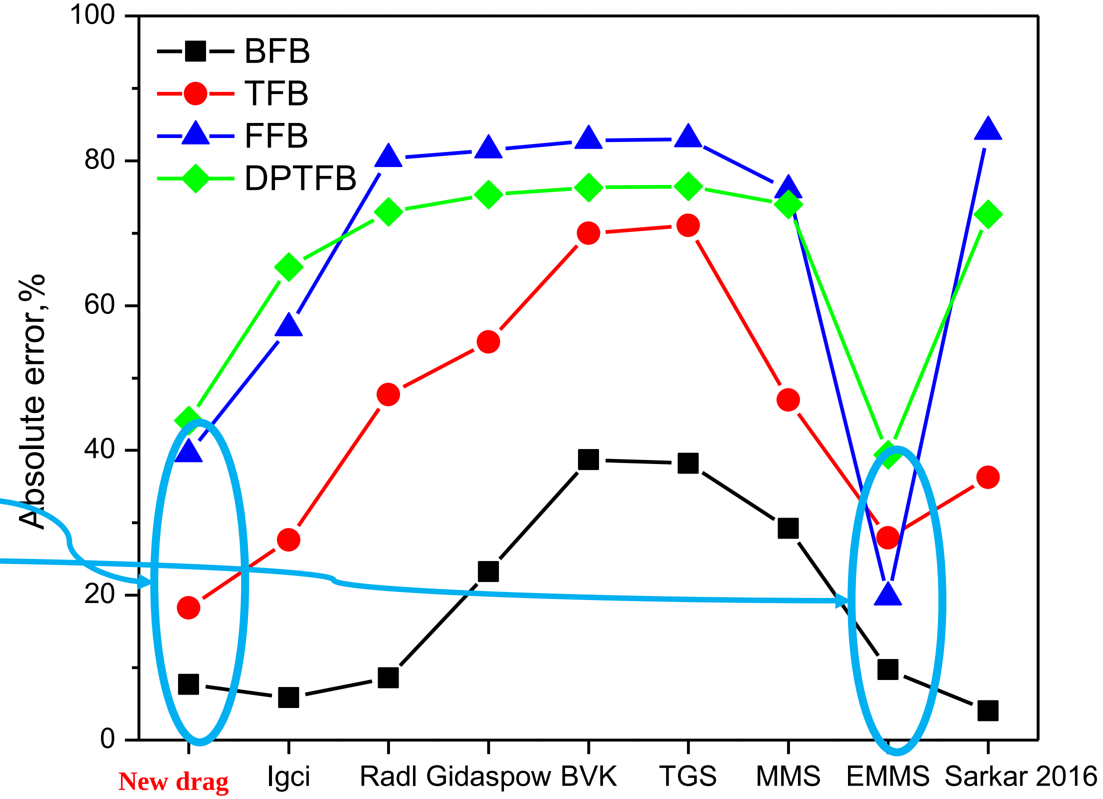
- Experimental measurements are pressure drop values
- Best agreement with heterogeneous drag models
  - (a) New drag
  - (h) EMMS (from literature)
- The old Sarkar (2016) drag model without a dense limit correction significantly under predicted the voidage.
- Ref: Andreux et al. (2008)

Determine Best Overall Drag Model

- **Evaluate the agreement for all fluidization regimes**
  - Define an average error

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

  - Based on this metric, the **new drag** model and the **EMMS drag** model yield the best agreement for all fluidization conditions



- The new drag model is a universal model, **hence it is one of the best options for gas-solid fluidized bed simulations**

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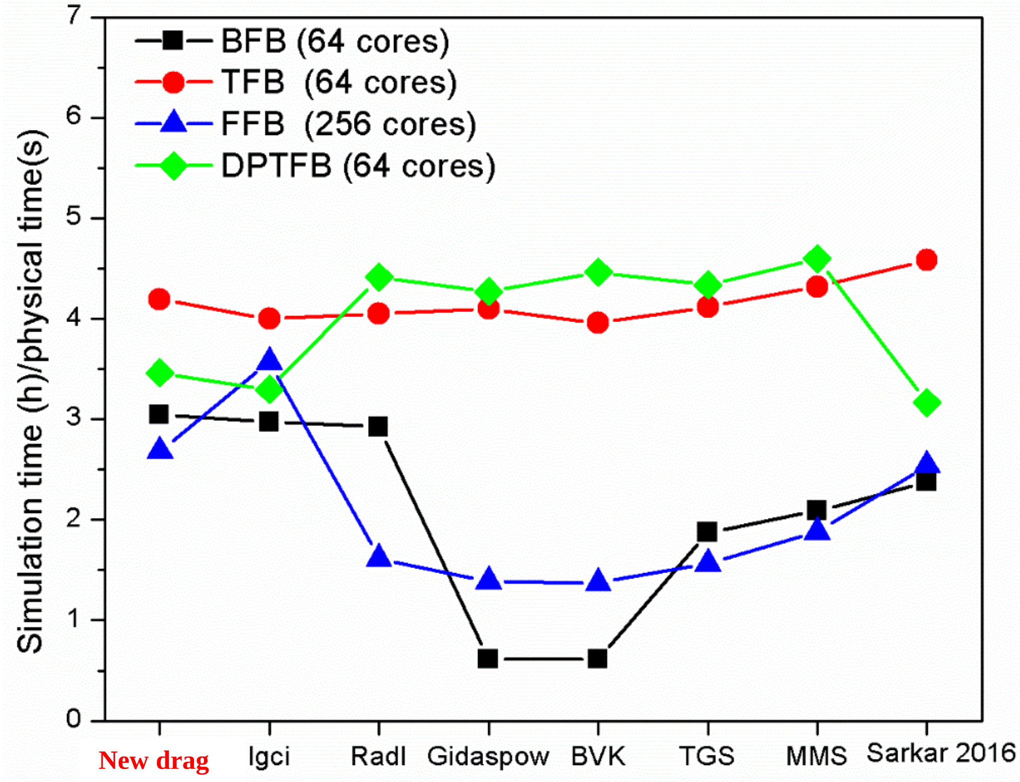
Comparison of Computational Cost

- **Evaluate the computational cost for all fluidization regimes**
  - Factors: complexity of the drag expression, the flow patterns simulated and the parallel efficiency
  - No significant difference in the TFB and DPTFB, about 4h/s.
  - The computational cost for some drag models (Gidaspow, BVK and TGS) are several times lower than the new drag model in BFB and FFB.
  - These drag models predicted significantly different flow patterns (overall less dense bed) compared with that predicted by the new drag model. (adaptive time step)



Summary of Results

- Coarse grid simulations with homogeneous drag models failed to capture the gas-solid fluidization behavior in all regimes. Modification of homogeneous drag models considering sub-grid effect is needed.

- A new filtered drag model was developed based on fine grid two fluid model simulation.

- The new drag model model gave superior predictions of the flow behavior in all fluidization regimes of Geldart A particles.

Acknowledgement

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Thanks for your attention!

Any Question?

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