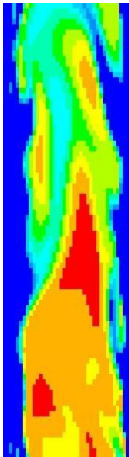


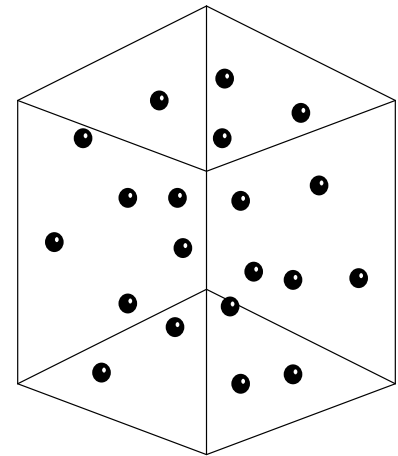
Multi-scale CFD Approach: Applied to Fluid Catalytic Cracking (FCC) Riser

Dr Milinkumar Shah

Department of Chemical Engineering
Curtin University, Bentley, Perth, WA



Curtin University



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'Nobody believed the result of a CFD calculation except the one who has generated it.'



'Perhaps today an appropriate statement would be that- Most of the people believe the result except the originator'



Curtin University

Outline

- Introduction
 - Computational fluid dynamics (CFD)
 - Multi-scale
- Case study: CFD of FCC riser
 - Gas-solid flow in riser
 - Challenges
 - Multi-scale darg model
 - Simulation results
- Summary

What is CFD?

Inlet fluid

- Material
- Velocity
- Temp.

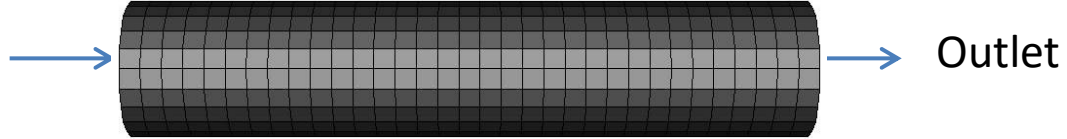


Required solution:
What will be the velocity field,
pressure profiles, temperature
distributions in flow domain?

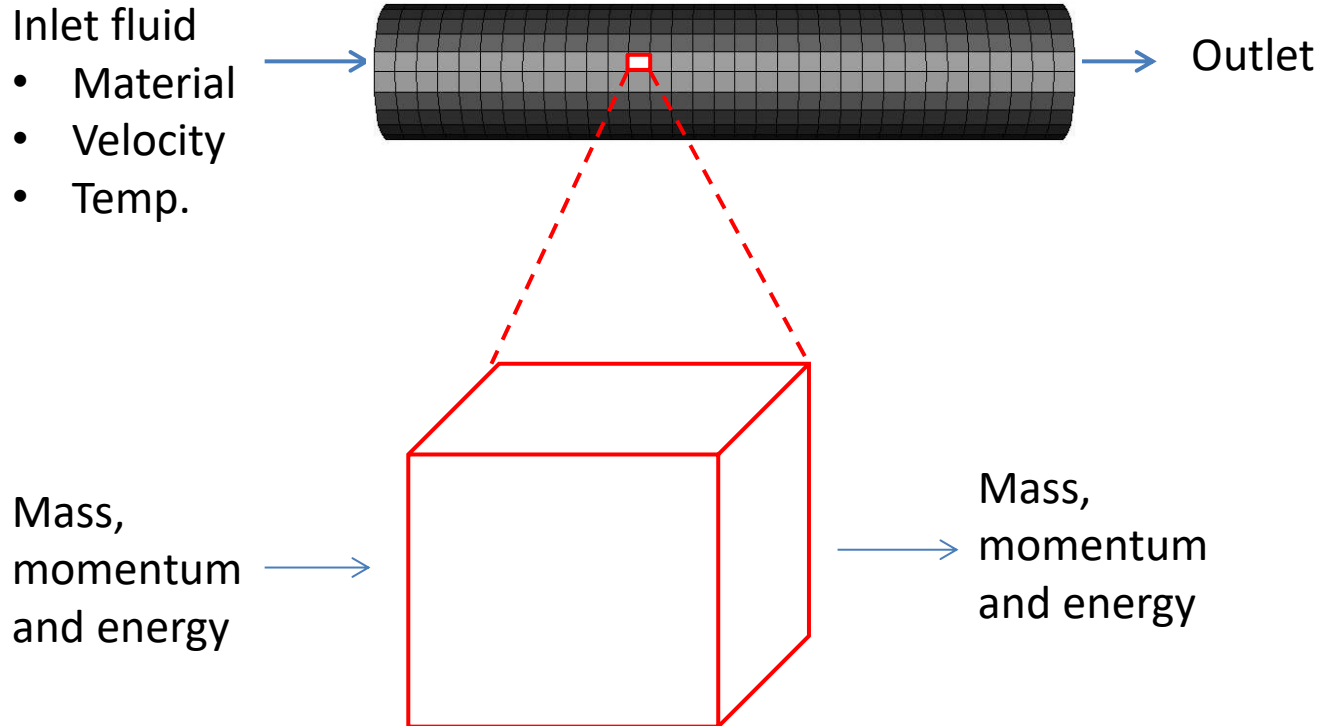
What is CFD?

Inlet fluid

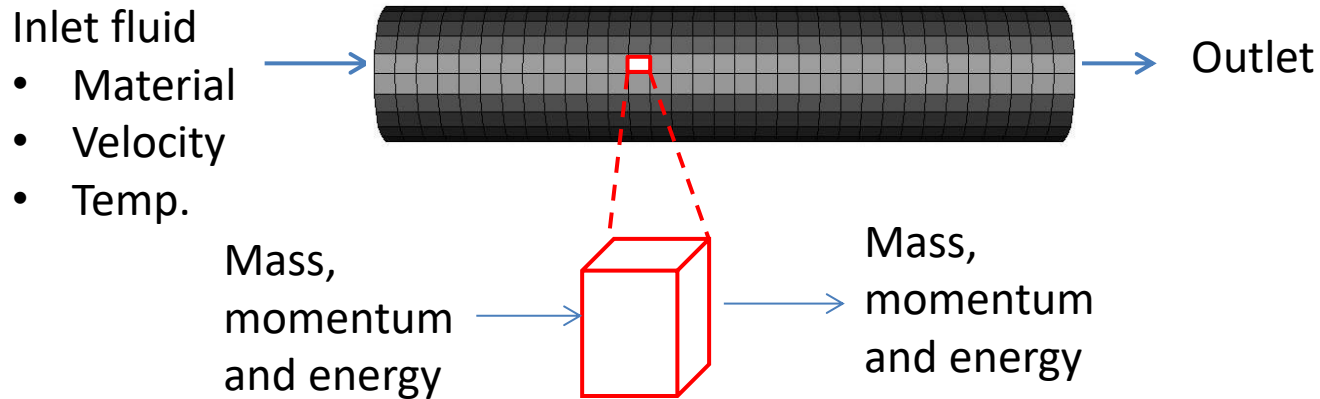
- Material
- Velocity
- Temp.



What is CFD?



What is CFD?



$$\text{Mass} \rightarrow \frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{u}) = 0 \text{ or } \frac{\partial(\rho)}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$

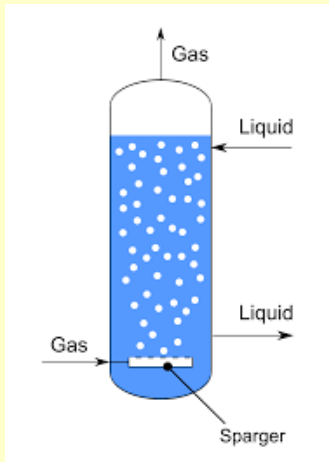
$$\text{x-momentum} \rightarrow \frac{\partial(\rho u)}{\partial t} + \text{div}(\rho u \mathbf{u}) = -\frac{\partial(p)}{\partial x} + \text{div}(\mu \text{grad} u) + S_{Mx}$$

$$\text{y-momentum} \rightarrow \frac{\partial(\rho v)}{\partial t} + \text{div}(\rho v \mathbf{u}) = -\frac{\partial(p)}{\partial y} + \text{div}(\mu \text{grad} v) + S_{My}$$

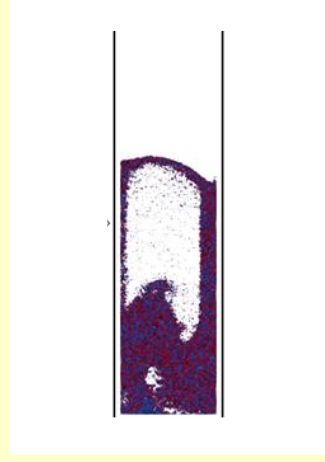
$$\text{z-momentum} \rightarrow \frac{\partial(\rho w)}{\partial t} + \text{div}(\rho w \mathbf{u}) = -\frac{\partial(p)}{\partial z} + \text{div}(\mu \text{grad} w) + S_{Mz}$$

Multi-scale: What and Why

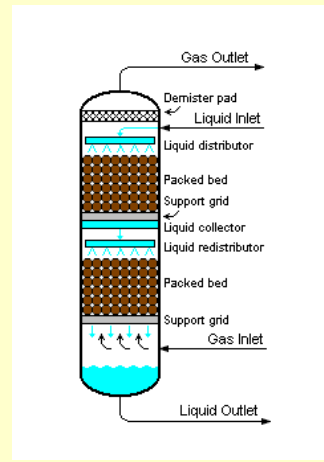
Multiphase reactors in chemical engineering



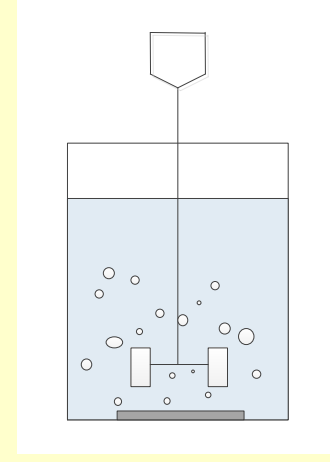
Bubble columns



Fluidized bed



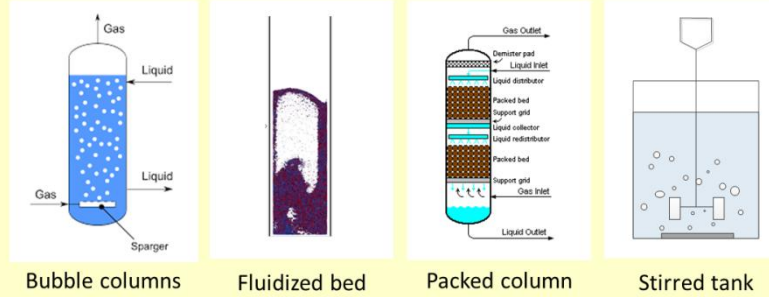
Packed column



Stirred tank

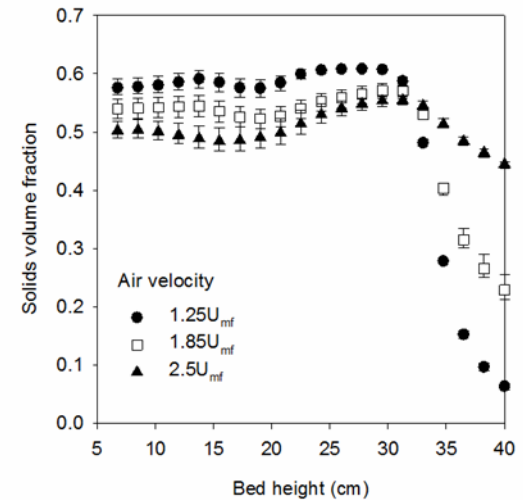
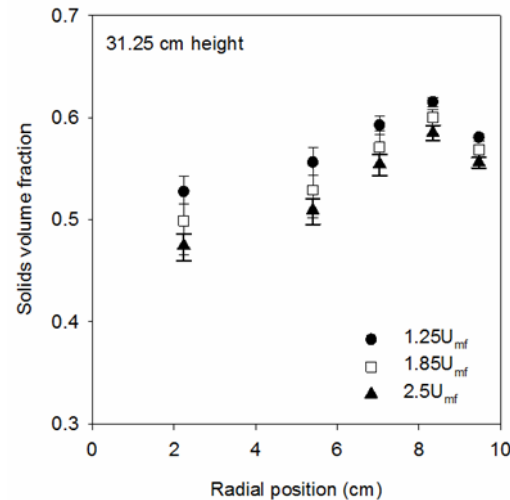
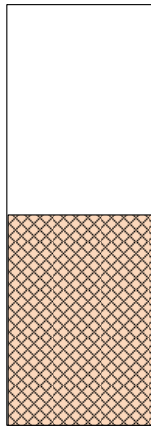
Multi-scale: What and Why

Multiphase reactors in chemical engineering



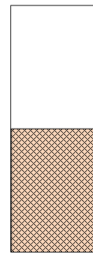
Example: Fluidized bed

Time-averaged solids volume fraction profiles

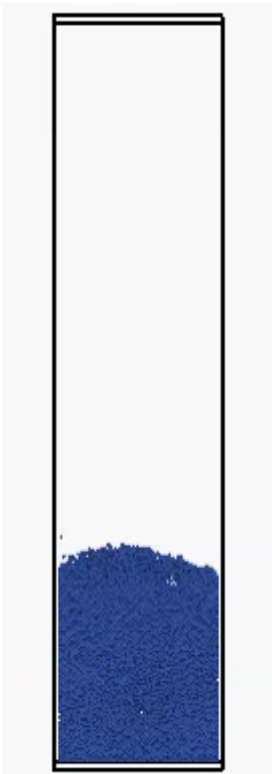
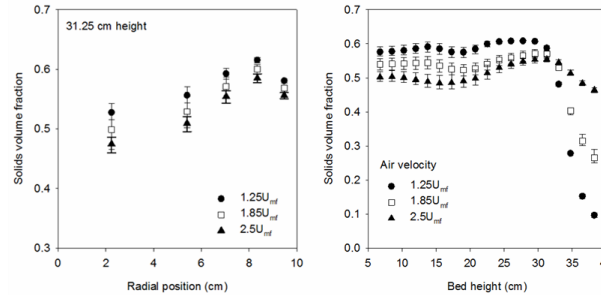


Multi-scale: What and Why

Example: Fluidized bed



Time-averaged solids volume fraction profiles

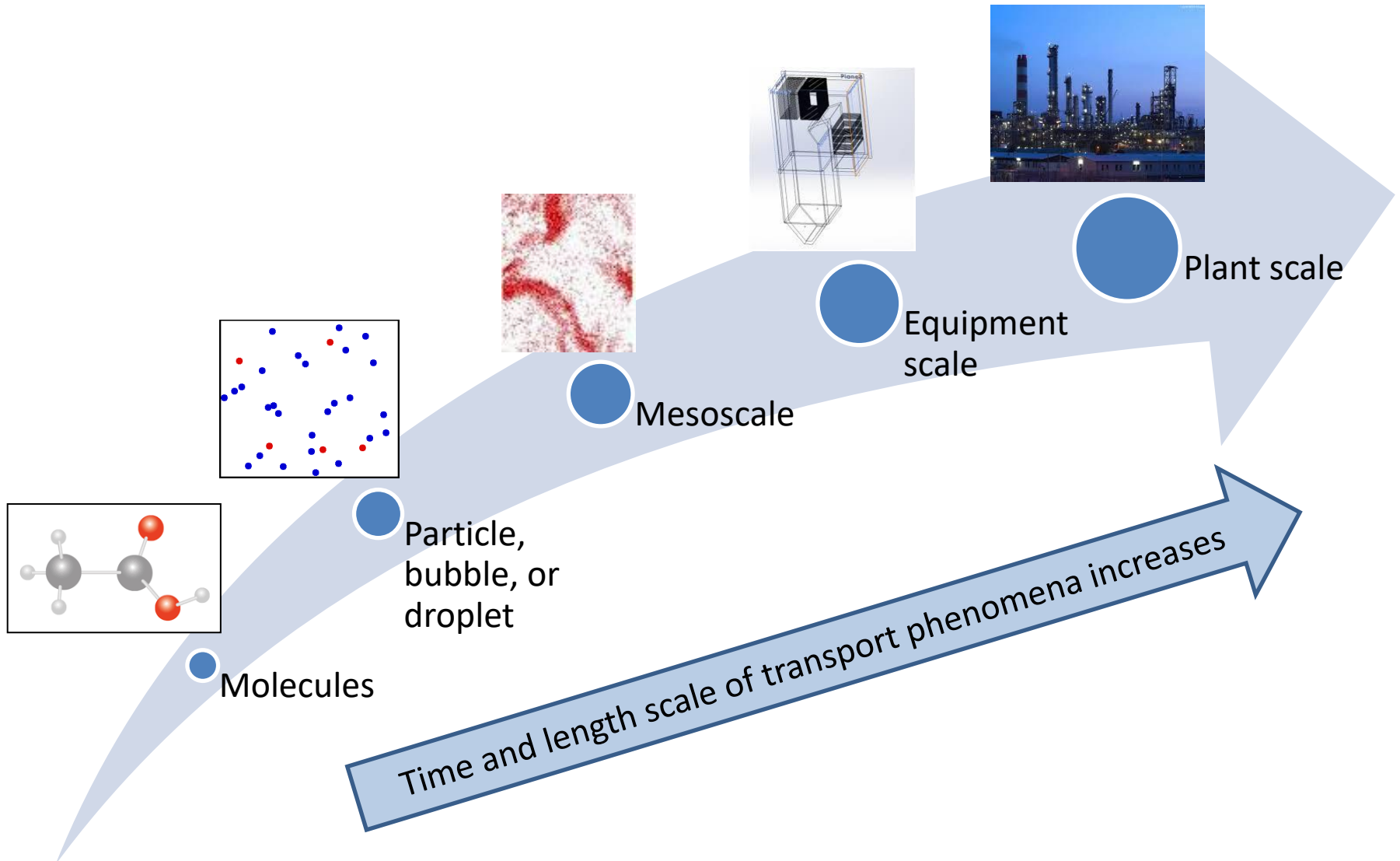


Bubble phenomena:

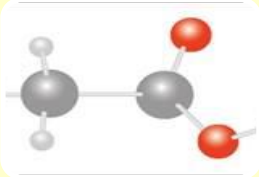
- Formation
- Coalescence
- Breakup
- Eruption

Time-scale: fraction of second
Length-scale: millimetre to centimetre

Multi-scale: What and Why

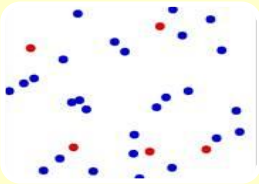


Multi-scale: What and Why



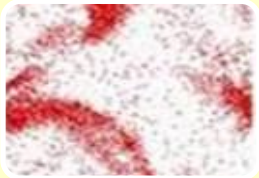
Molecular scale

- Molecular modelling



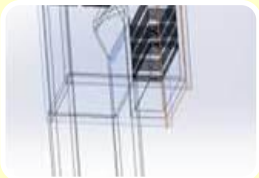
Particle scale

- Direct numerical simulations



Meso scale

- Very fine grid CFD simulations



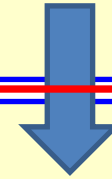
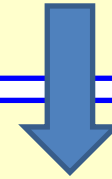
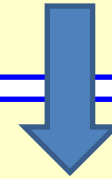
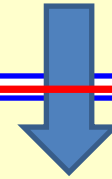
Equipment scale

- Coarse grid CFD simulations



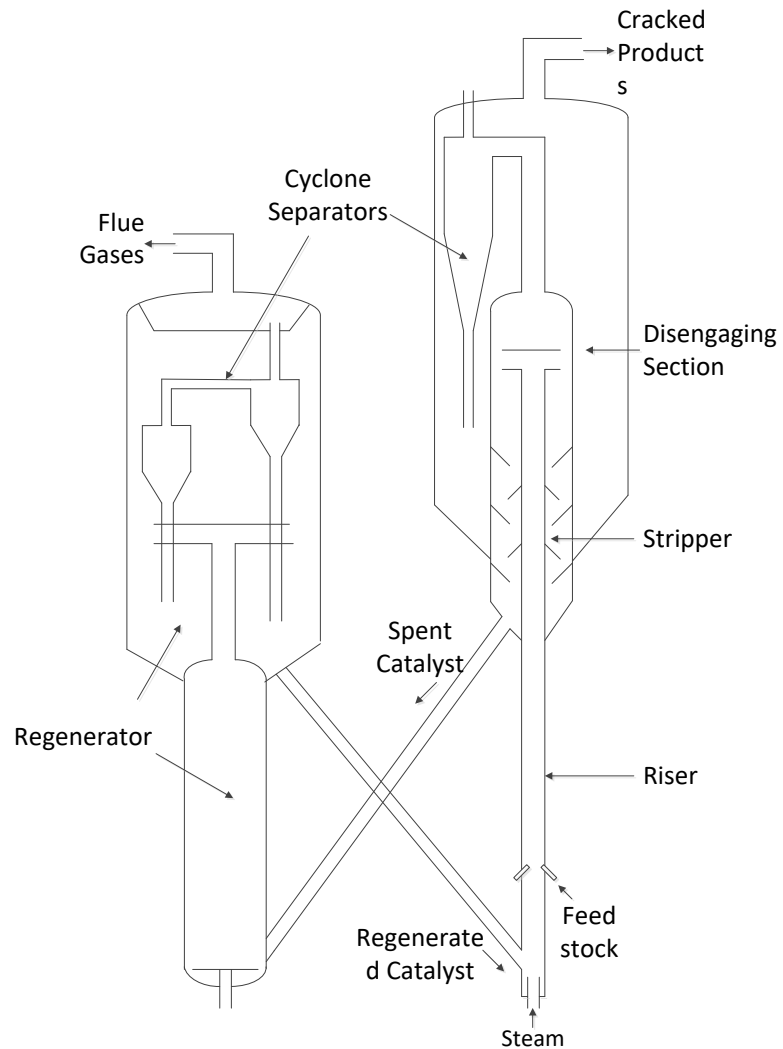
Plant scale

- Flow sheet simulations

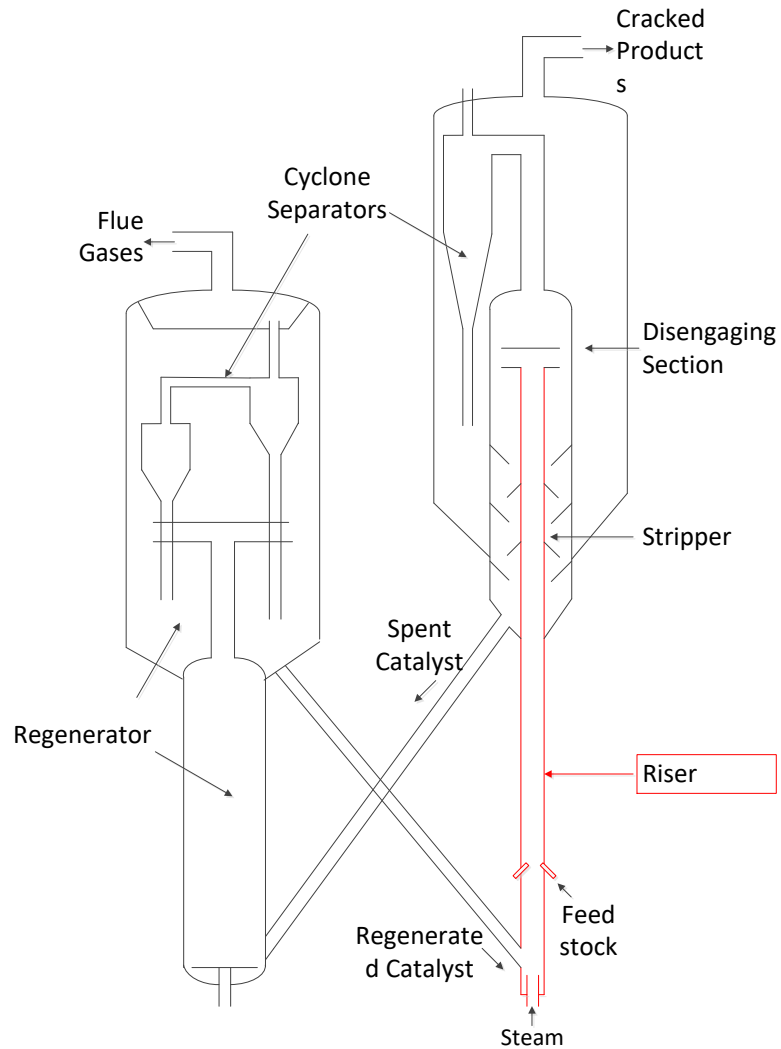


Case study:
Multiscale approach for CFD
simulations of fluid catalytic cracking
riser

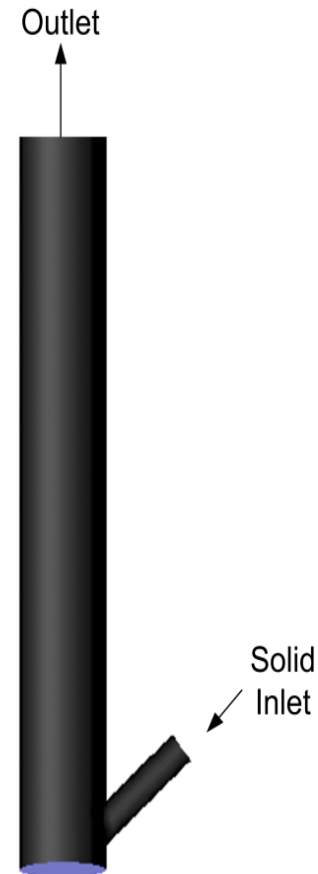
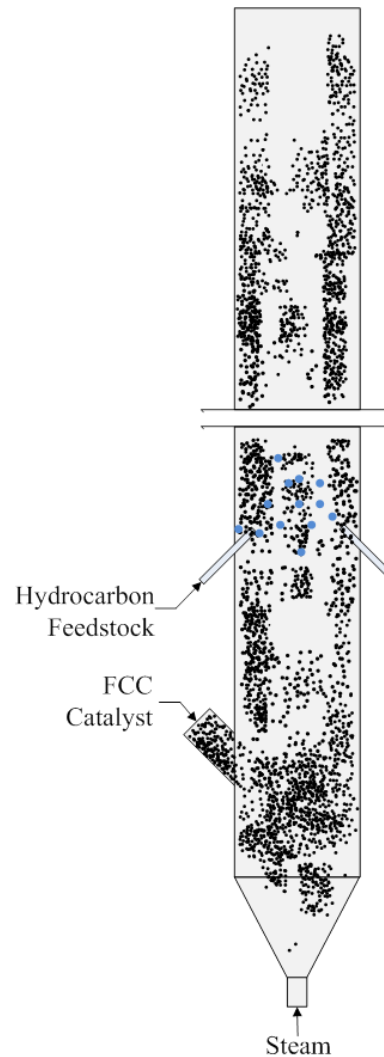
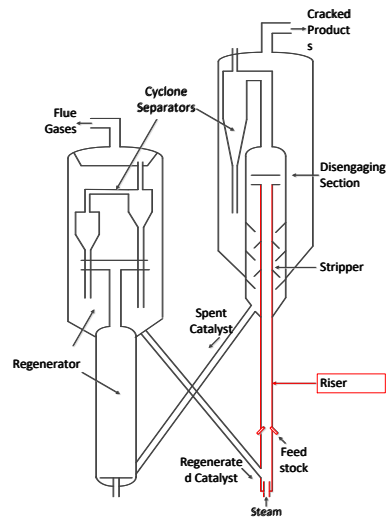
Case study: FCC riser



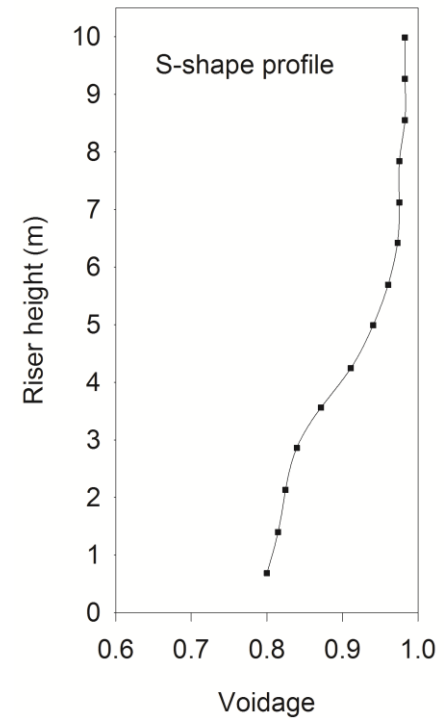
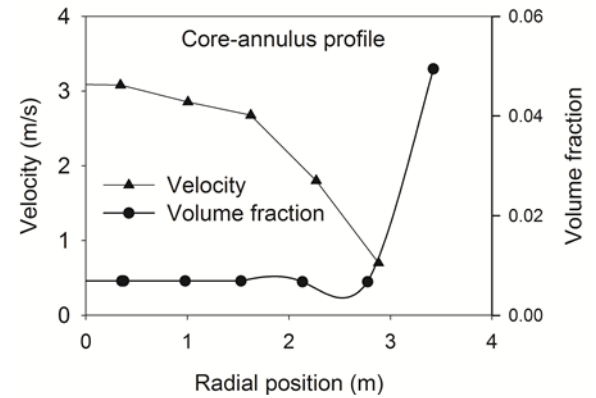
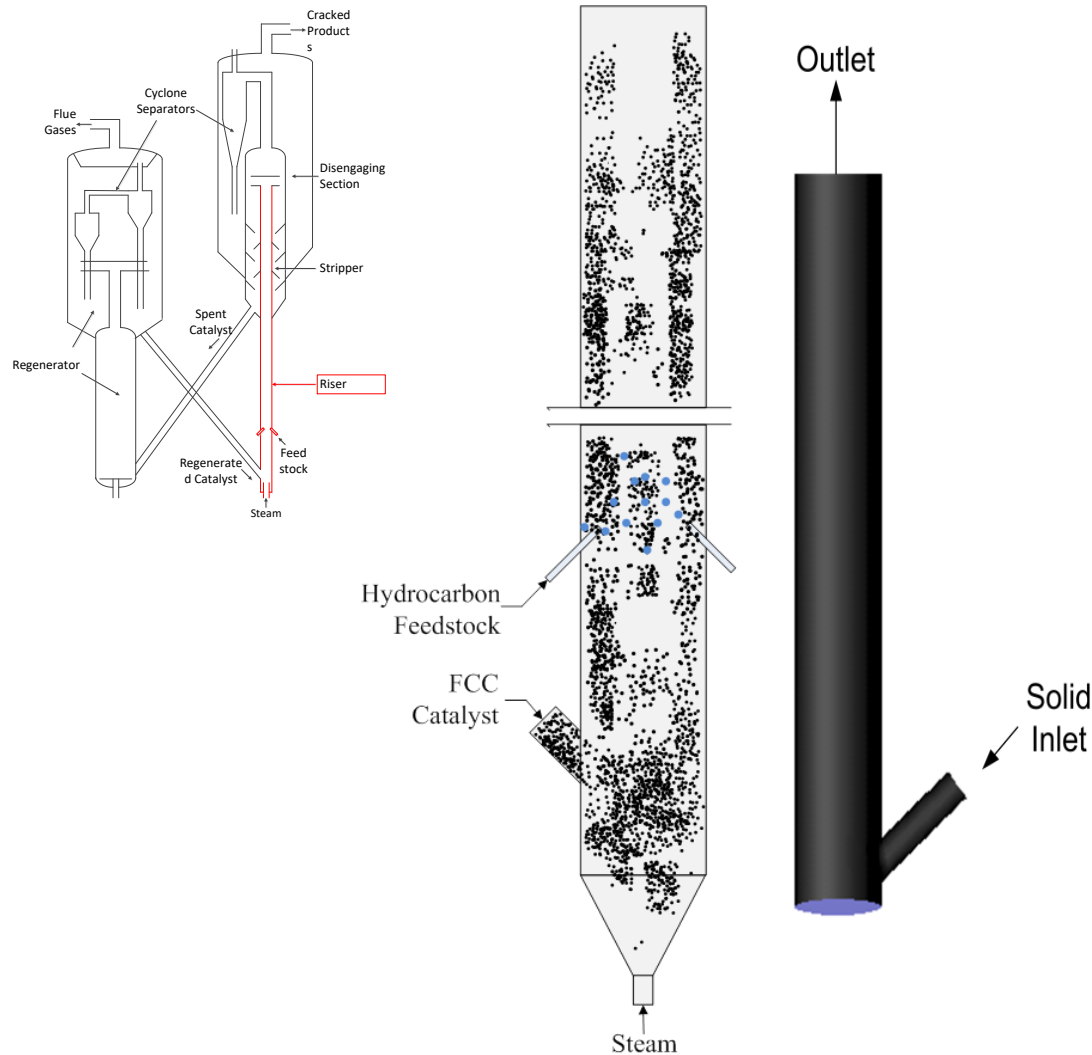
Case study: FCC riser



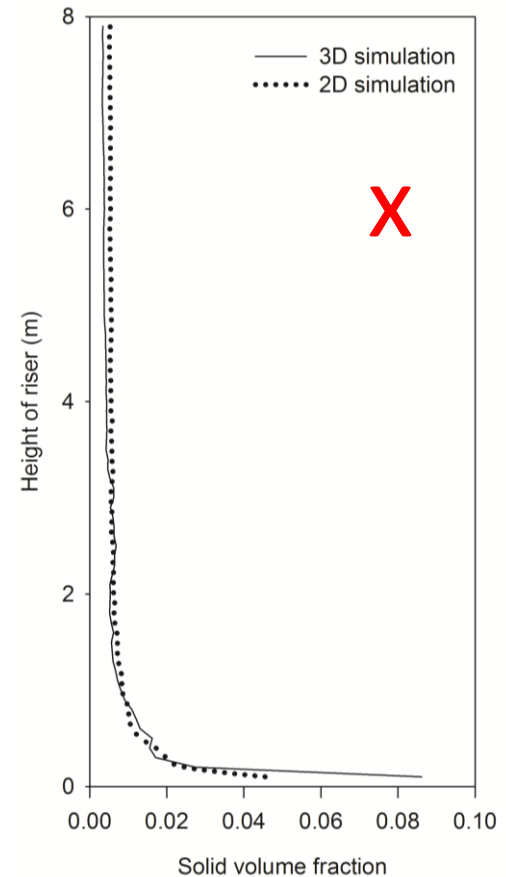
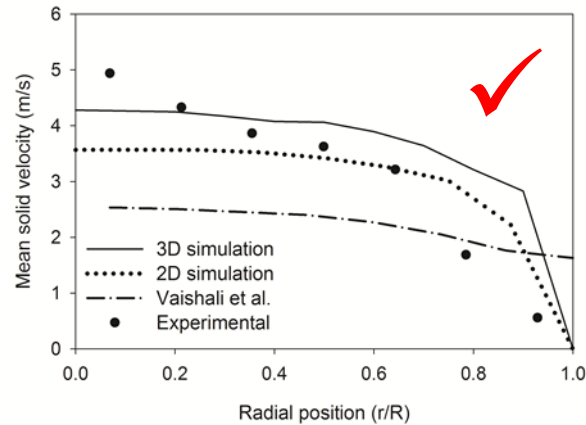
Case study: FCC riser



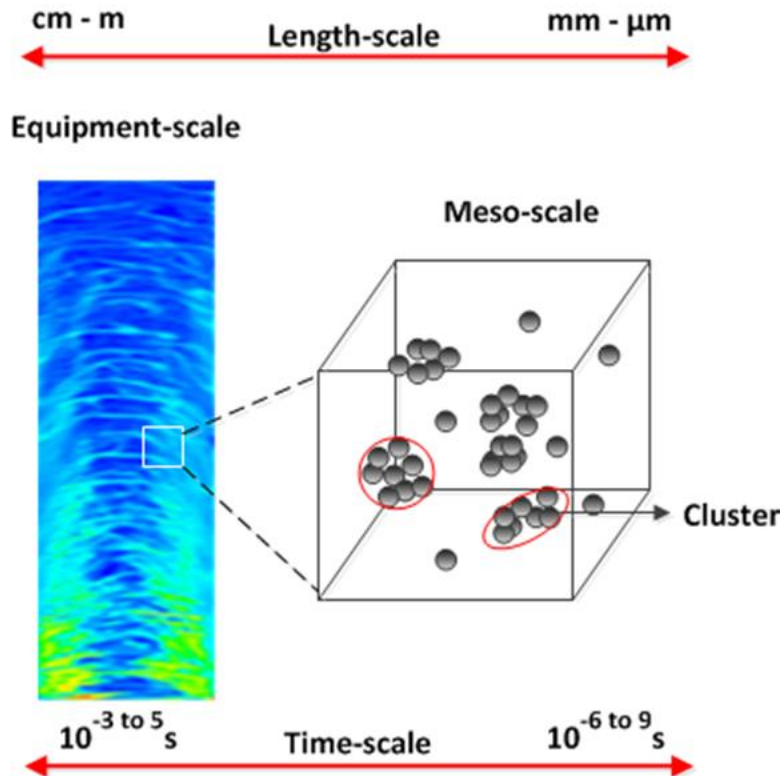
Case study: FCC riser



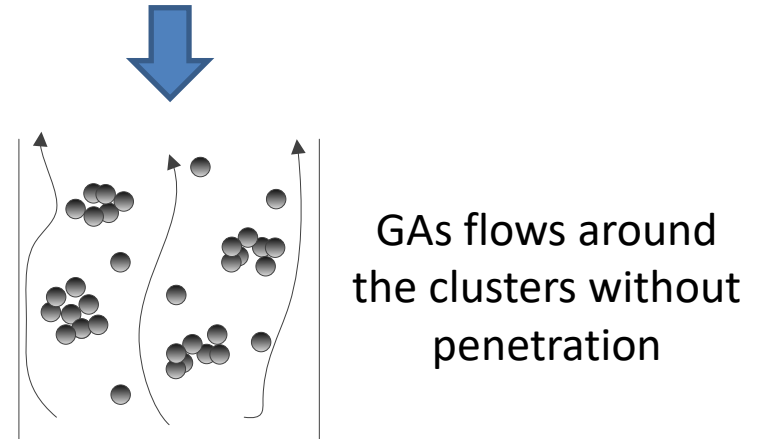
Challenges in CFD simulations



Challenges in CFD simulations

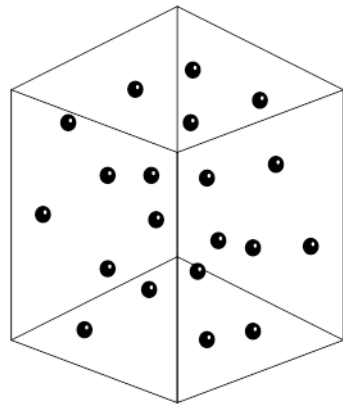


Formation of Clusters

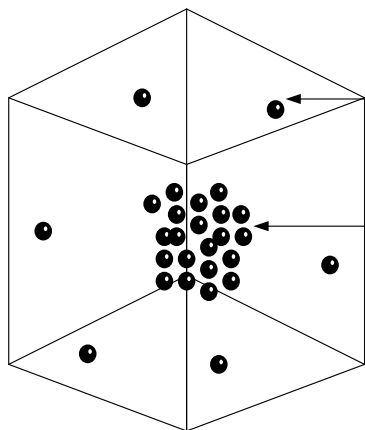
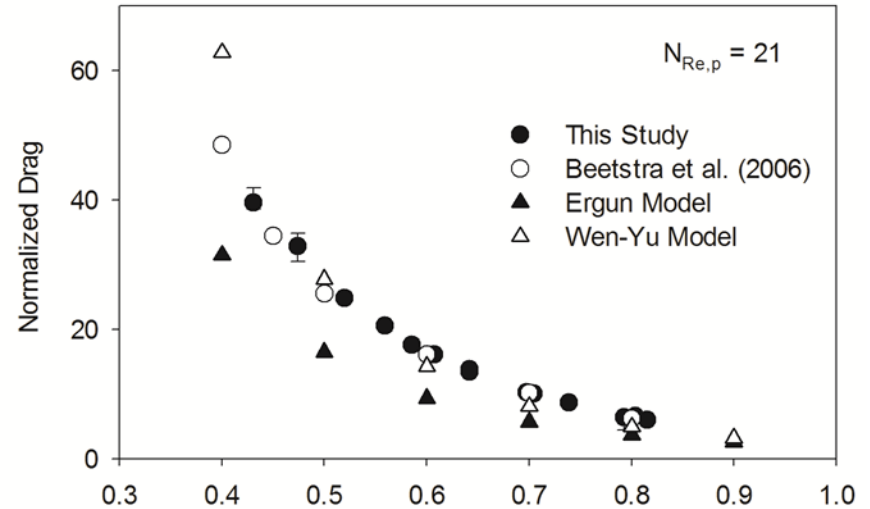


Significant Drag Reduction

Effect of a cluster on gas-solid drag



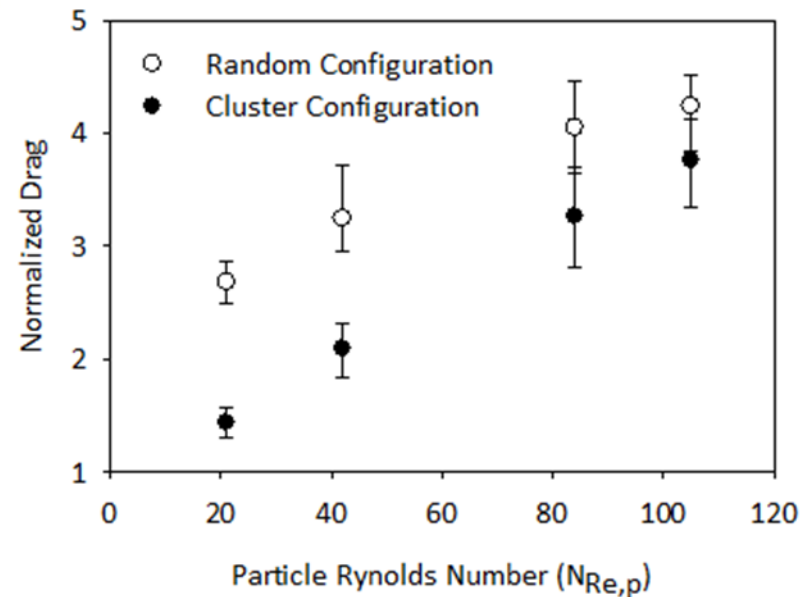
Particles at
random positions



Surrounding
Individual Particle

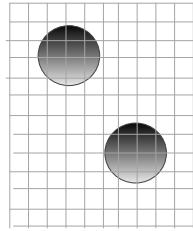
Cluster

Boundaries of
Cubical Flow Domain



How to account for clusters in drag

Sub Grid Scale Approach



Fine grid periodic simulations

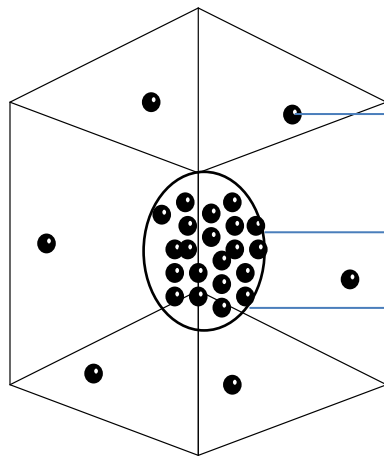
Energy minimization
multiscale (EMMS)
Approach



Drag is derived by local flow conditions + empirically calculated cluster diameter

EMMS Approach

EMMS divides flow in three pseudo phases



Individual particles in dilute phase

Particles in dense cluster phase

Individual cluster as a large particle

Apply conventional Wen-Yu model to calculate gas-solid drag in each pseudo phase

EMMS Approach

$$m_f F_f = \left[\frac{(1-f)(1-\varepsilon_f)}{\frac{\pi}{6} d_p^3} \right] \left[C_{Df} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sf}^2 \right] \quad \text{Drag on particles in dilute phase}$$

$$m_c F_c = \left[\frac{f(1-\varepsilon_c)}{\frac{\pi}{6} d_p^3} \right] \left[C_{Dc} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sc}^2 \right] \quad \text{Drag on particles in cluster phase}$$

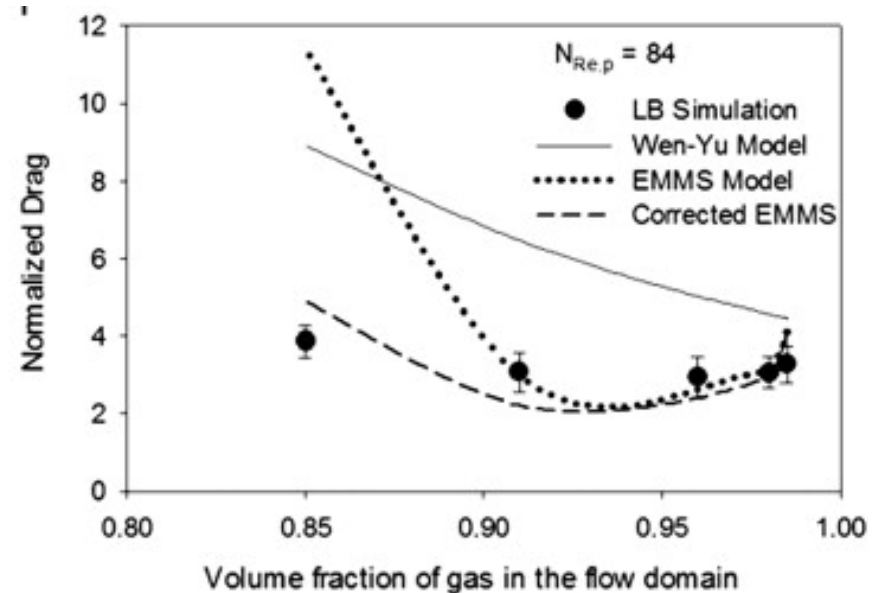
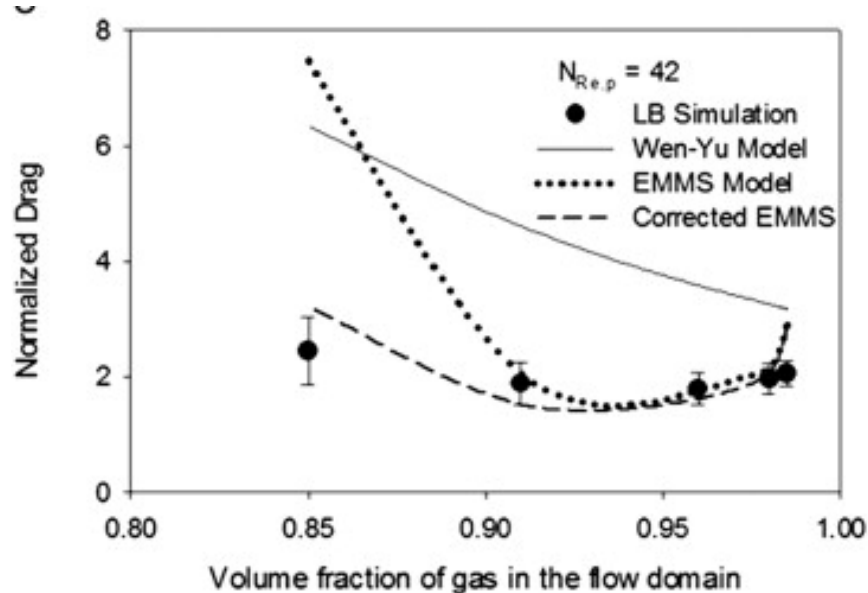
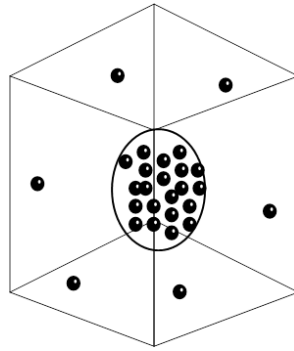
$$m_i F_i = \left[\frac{f}{\frac{\pi}{6} d_{cl}^3} \right] \left[C_{Di} \frac{\pi}{4} d_{cl}^2 \frac{\rho_f}{2} U_{si}^2 \right] \quad \text{Drag on clusters}$$

$$C_{D,Wen-Yu} = C_{D0} \varepsilon^{-4.7} \text{ and } C_{D0} = \frac{24}{Re,p} (1 + 0.15 Re,p^{0.687})$$

$$F_D = (m_c F_c + m_f F_f + m_i F_i)$$

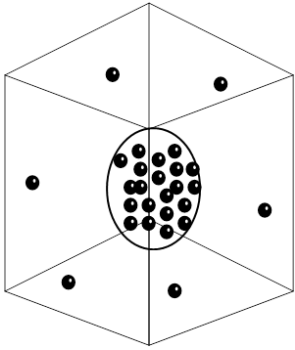
c = cluster; f = dilute phase; i = dense phase; ε = voidage; U_s = superficial slip velocity; m_c , m_f and m_i = number of particles per unit volume in cluster, dilute and dense phases; F_c , F_f and F_i = force per unit volume in cluster, dilute and dense phases

Verification of EMMS Approach



Drag from EMMS approach and LBM simulations compares well for flow through cluster configuration at particle Reynolds numbers ranging from 21-105

EMMS Approach

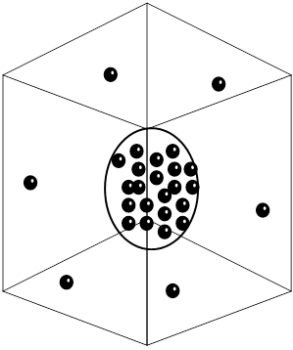


How to calculate diameter of clusters?

What is void fraction inside clusters?

How to calculate slip velocities in three pseudo phases?

EMMS Approach



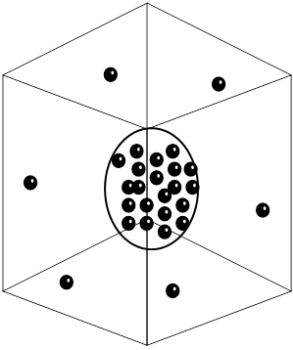
What is diameter of clusters?

Empirical equations are available which correlates cluster diameter with overall void fraction.

What is void fraction inside clusters?

How to calculate slip velocities for three pseudo phases?

EMMS Approach



How to calculate diameter of clusters?

Empirical equations are available which correlates cluster diameter with overall void fraction.

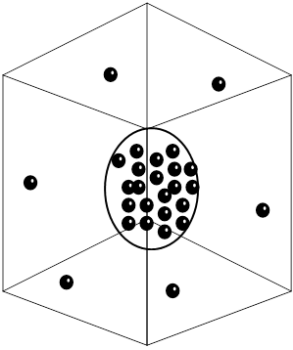
How to calculate void fraction inside clusters?

Can be arbitrarily selected as 0.7

This is an intermediate voidage between that at maximum packing limit (0.63) and completely dilute flow (1)

How to calculate slip velocities for three pseudo phases?

EMMS Approach



How to calculate diameter of clusters?

Empirical equations are available which correlates cluster diameter with overall void fraction.

How to calculate void fraction inside clusters?

The value of 0.7 can be used.

This value is an intermediate voidage between that at maximum packing limit (0.63) and completely dilute flow (1)

How to calculate slip velocities in three pseudo phases?

The slip velocities can be calculated from mass and pressure balance equations for each pseudo phases.

EMMS Approach

$\varepsilon = \varepsilon_c f + \varepsilon_f (1 - f)$ ➡ Overall mass balance equation

$U_p = U_{pc} f + U_{pf} (1 - f)$ ➡ Mass balance of particle phase

$U_g = U_c f + U_f (1 - f)$ ➡ Mass balance of gas phase

ε_f can be assumed to be 1 (completely dilute phase).

If $\varepsilon_f = 1$ (no particles), then $U_{pf} = 0$ and $U_{pc} = U_p / f$

U_g and U_p are superficial gas and particle velocities

$$U_f = \frac{U_g - \frac{\varepsilon_c}{(1 - \varepsilon_c)} U_p}{1 - f} - \frac{f}{1 - f} U_{sc}$$

$$U_c = \frac{\varepsilon_c}{(1 - \varepsilon_c)} U_{pc} + U_{sc}$$

EMMS Approach

Force balance for particles in dense phase:

$$\frac{f(1-\varepsilon_c)}{\frac{\pi}{6}d_p^3} C_{Dc} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sc}^2 + \frac{f}{\frac{\pi}{6}d_{cl}^3} C_{Di} \frac{\pi}{4} d_{cl}^2 \frac{\rho_f}{2} U_{si}^2 = f(1-\varepsilon_c)(\rho_p - \rho_f)(g + a)$$

Force balance for particles in dilute phase

$$\frac{(1-f)(1-\varepsilon_f)}{\frac{\pi}{6}d_p^3} C_{Df} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sf}^2 = (1-f)(1-\varepsilon_f)(\rho_p - \rho_f)(g + a)$$

Pressure balance

$$\Delta P_{dilute} + \frac{m_i F_i}{(1-f)} = \Delta P_{dense}$$

$$m_f F_f + \frac{m_i F_i}{(1-f)} = m_c F_c$$

$$\frac{(1-\varepsilon_f)}{\frac{\pi}{6}d_p^3} C_{Df} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sf}^2 + \frac{f}{(1-f)\frac{\pi}{6}d_{cl}^3} C_{Di} \frac{\pi}{4} d_{cl}^2 \frac{\rho_f}{2} U_{si}^2 = \frac{f(1-\varepsilon_c)}{\frac{\pi}{6}d_p^3} C_{Dc} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sc}^2$$

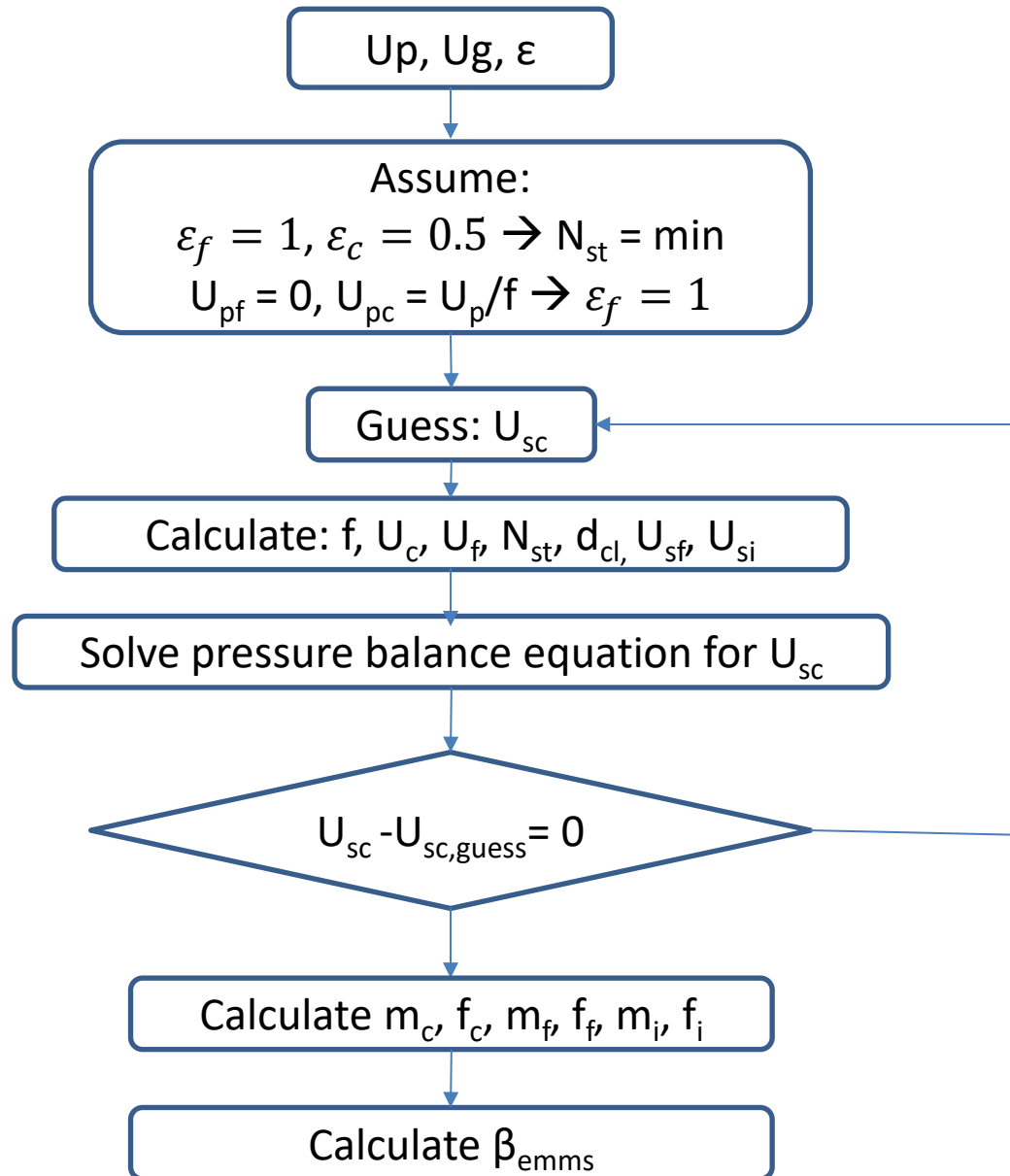
EMMS Approach

From force balances and pressure balance equations, along with mass balances, following two algebraic equations can be derived.

$$0.15 \left(\frac{\rho_f d_{cl}}{\mu_f} \right)^{0.687} \left[\left(U_f - \frac{\varepsilon_f}{1 - \varepsilon_c} U_{pc} \right) (1 - f) \right]^{1.687} + \left[\left(U_f - \frac{\varepsilon_f}{1 - \varepsilon_c} U_{pc} \right) (1 - f) \right] \\ - (1 - f)^{5.7} (\varepsilon_f - \varepsilon_c) \frac{(\rho_p - \rho_f)}{18\mu_f} (g + a) d_{cl}^2 = 0$$

$$0.15 \left(\frac{\rho_f d_{cl}}{\mu_f} \right)^{0.687} U_{sc}^{1.687} + U_{sc} - \frac{[(1 - \varepsilon_f) + (\varepsilon_f - \varepsilon_c)] \varepsilon_c^{-4.7} (\rho_p - \rho_f) (g + a) d_p^2}{1 - \varepsilon_c} \frac{1}{18\mu_f} = 0$$

EMMS Approach



EMMS Approach

Energy consumed in suspending and transporting particles

$$N_{st} = \frac{1}{(1 - \varepsilon)\rho_p} (m_c F_c U_c f + m_f F_f U_f (1 - f) + m_i F_i U_f (1 - f))$$

$$N_{st} = \left[U_g - \frac{\varepsilon_f - \varepsilon}{1 - \varepsilon} f (1 - f) U_f \right] g \frac{\rho_p}{\rho_p - \rho_g} \quad \longrightarrow \quad \text{Li and Kwauk (1994)}$$

N_{st} becomes minimum when $\varepsilon_f = 1$ and $\varepsilon_c = 0.7$ (Assumption)

Cluster diameter

$$d_{cl} = \frac{d_p \left(\frac{U_p g}{(1 - \varepsilon_{max})} - \left(U_{mf} + \frac{U_p \varepsilon_{mf}}{(1 - \varepsilon_{mf})} \right) g \right)}{N_{st} \frac{\rho_p}{\rho_p - \rho_g} \left(U_{mf} + \frac{U_p \varepsilon_{mf}}{(1 - \varepsilon_{mf})} \right) g} \quad \longrightarrow \quad \text{Empirical equation by Chavan (1984)}$$

EMMS Approach

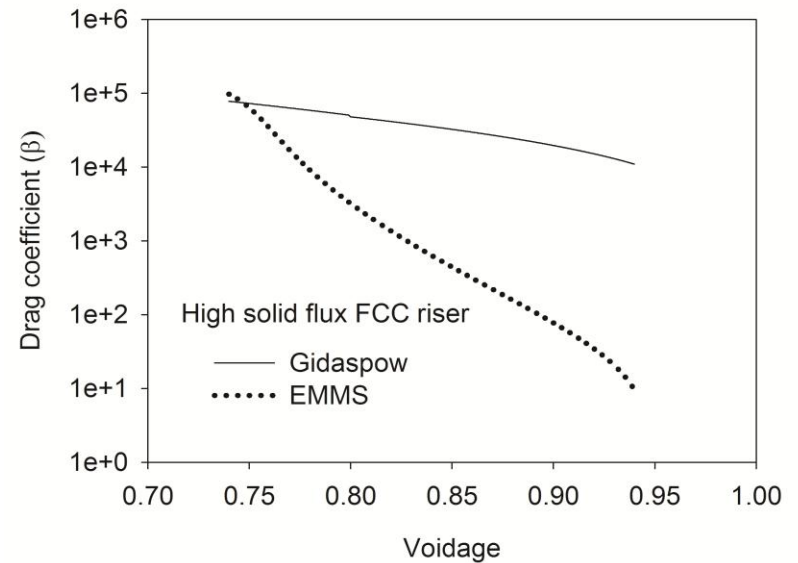
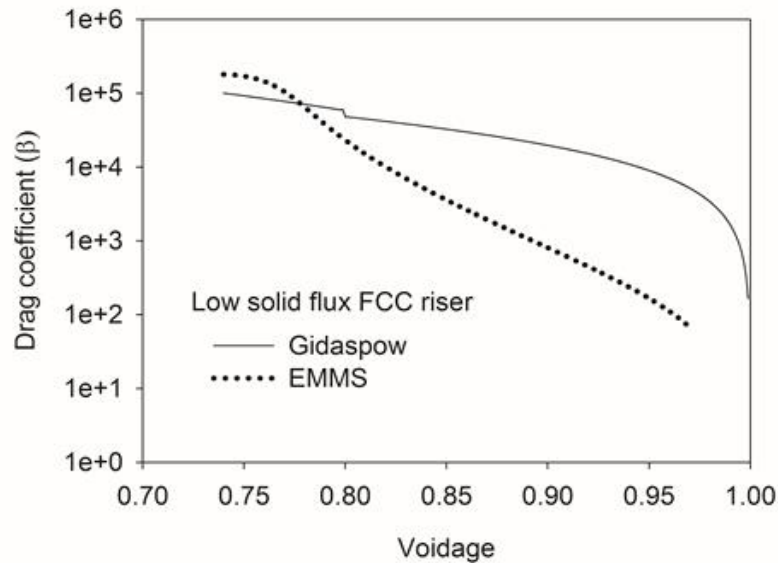
- Yang et al. (2003)

$$\frac{f(1-\varepsilon_c)}{\frac{\pi}{6}d_p^3} C_{Dc} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sc}^2 + \frac{f}{\frac{\pi}{6}d_{cl}^3} C_{Di} \frac{\pi}{4} d_{cl}^2 \frac{\rho_f}{2} U_{si}^2 = f(1-\varepsilon_c)(\rho_p - \rho_f)(g + a)$$

$$\frac{(1-f)(1-\varepsilon_f)}{\frac{\pi}{6}d_p^3} C_{Df} \frac{\pi}{4} d_p^2 \frac{\rho_f}{2} U_{sf}^2 = (1-f)(1-\varepsilon_f)(\rho_p - \rho_f)(g + a)$$

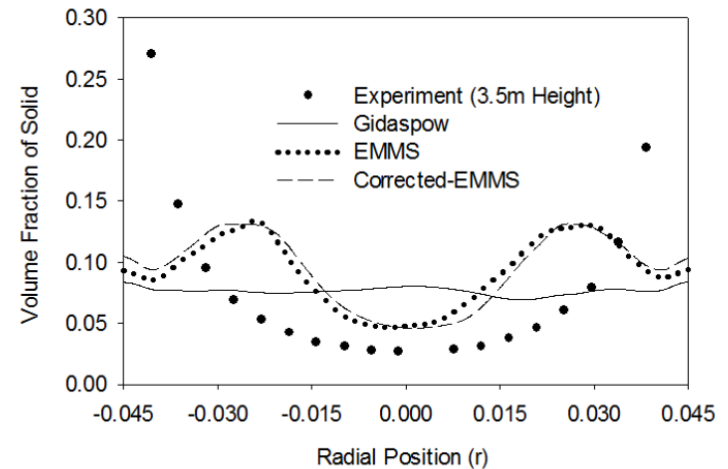
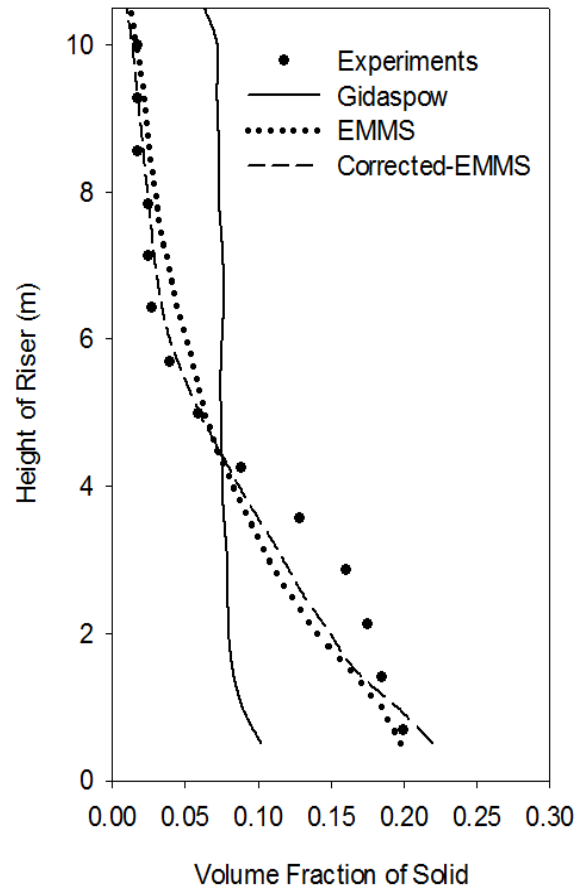
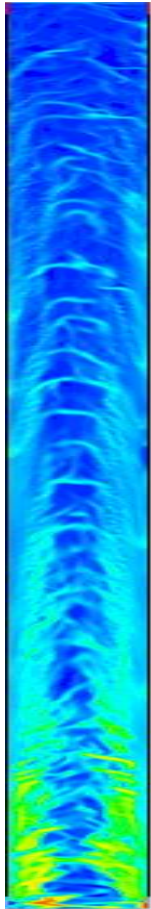
- Here, there are two unknowns U_{sc} and a , which can be calculated by two algebraic equations.
 - Yang et al. (2003) assumes cluster voidage to be 0.7 instead of 0.5.
-
- Wang et al. (2007)
 - This version uses local velocities of U_g and U_p to derive EMMS drag values in each cell.

EMMS Drag

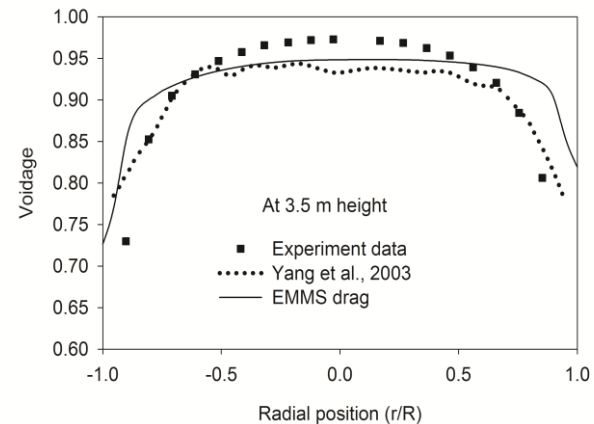
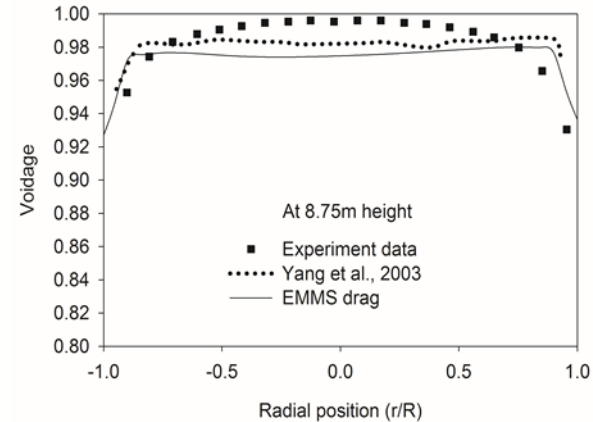
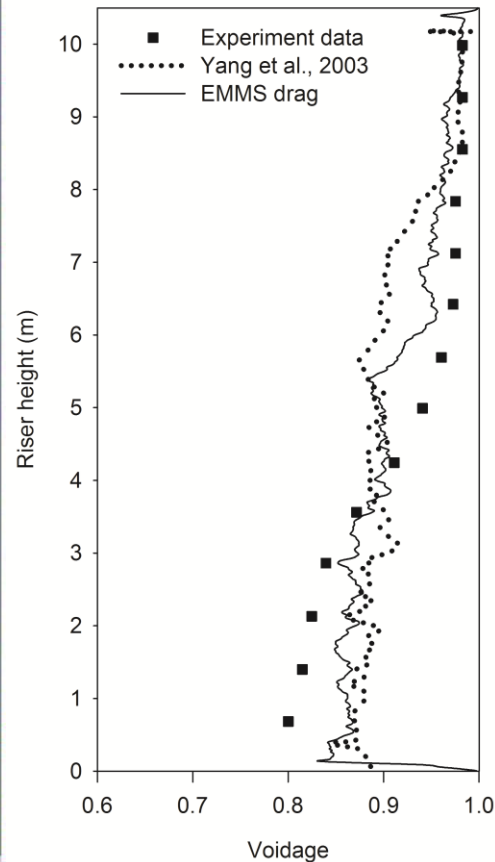
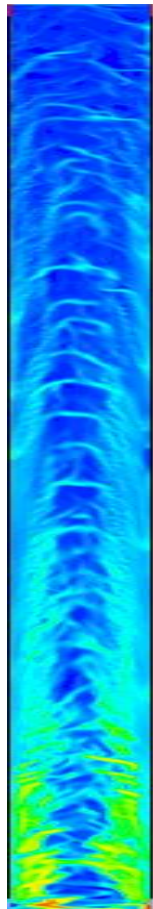


	Low solid flux	High solid flux
Particle dia. (d_p)	54 μm	76 μm
Density	930 kg/m^3	1712 kg/m^3
Solid mass flux (G_s)	14.3 $\text{kg/m}^2\text{s}$	489 $\text{kg/m}^2\text{s}$
Superficial gas velocity (U_g)	1.52 m/s	5.2 m/s

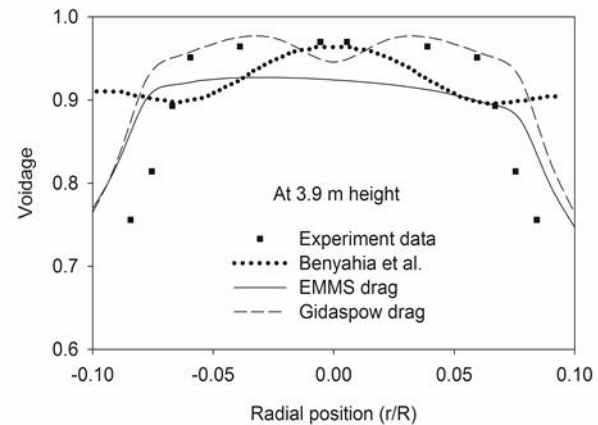
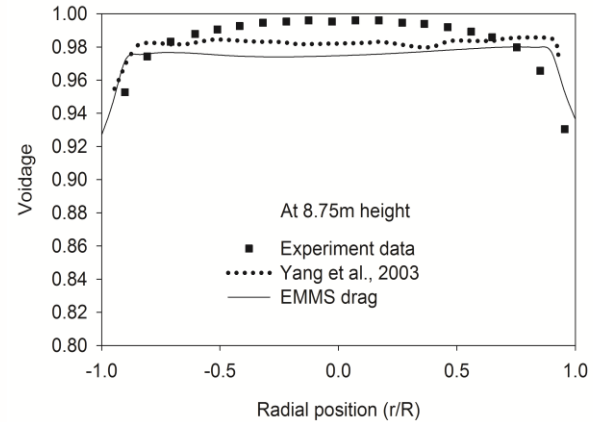
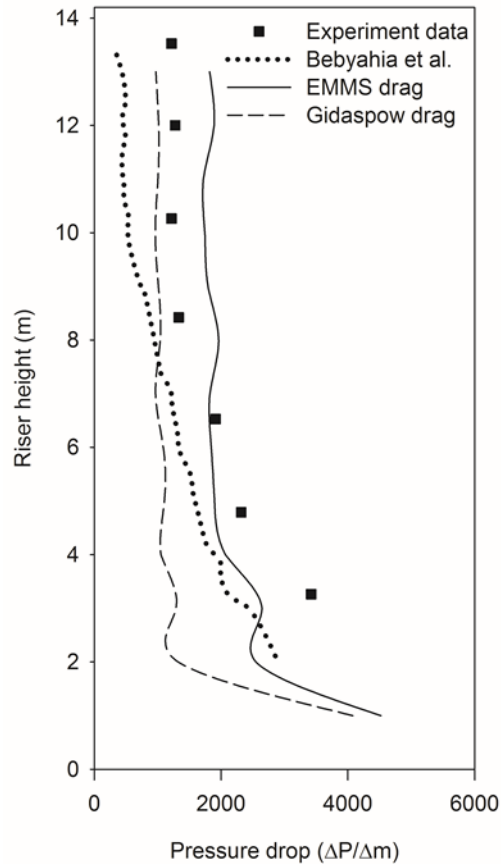
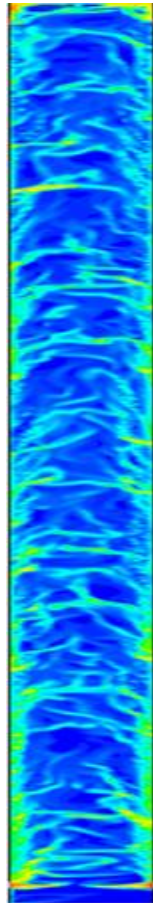
Use of EMMS: Riser simulations



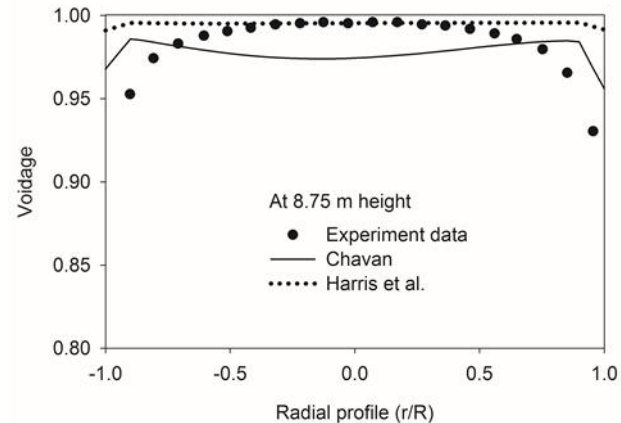
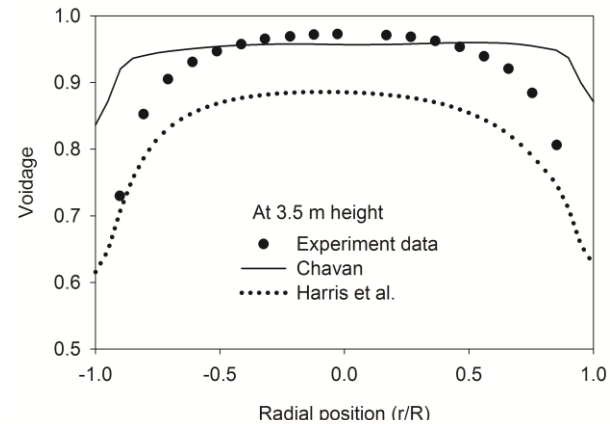
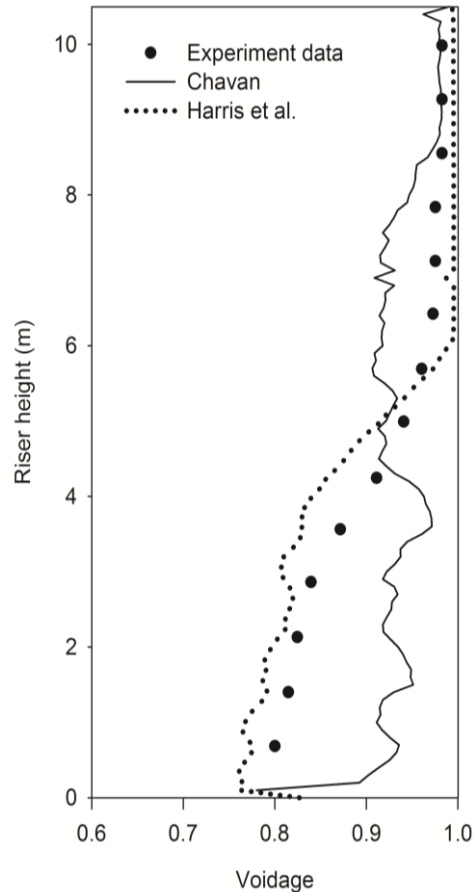
Use of EMMS: Riser simulations



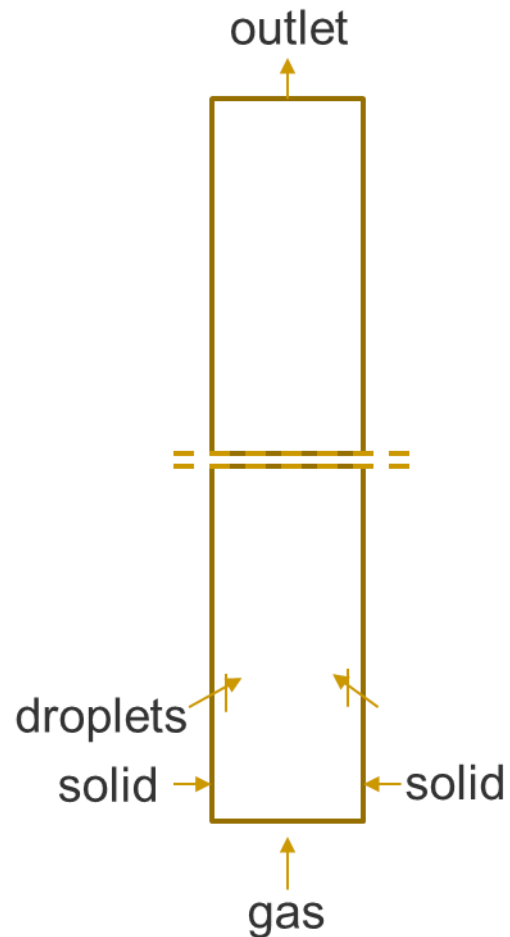
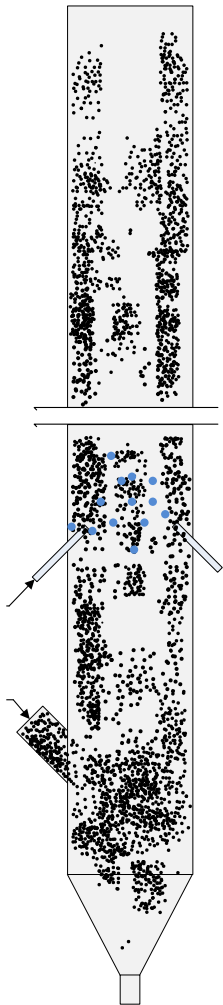
Use of EMMS: Riser simulations



Use of EMMS: Riser simulations

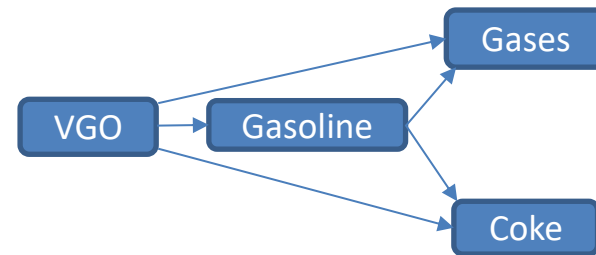


CFD of FCC Riser

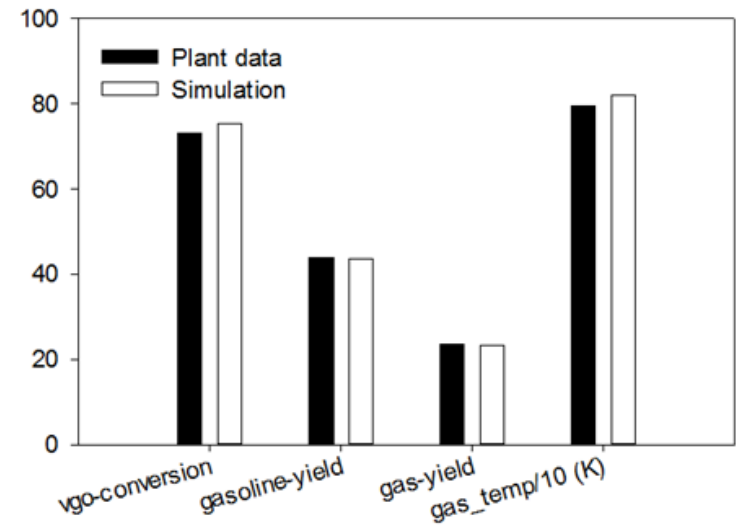
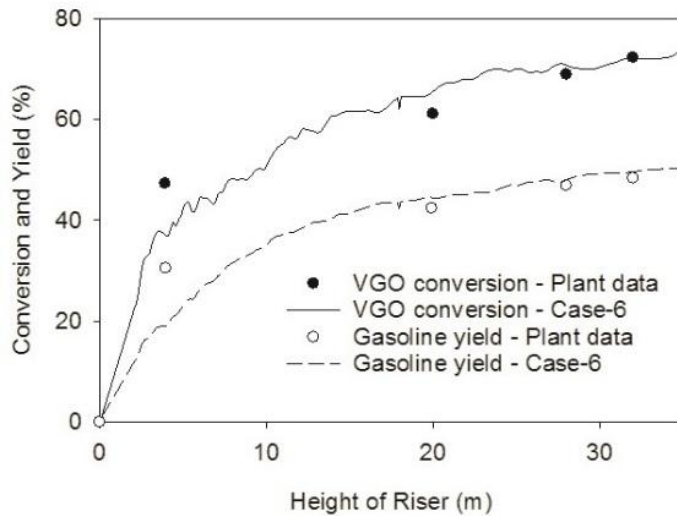


2D CFD model
Eulerian-Eulerian

4-lumps kinetic model (Lee et al., 1988)



CFD of FCC Riser



CFD model for FCC riser:

At mesoscale, EMMS approach was verified

At equipment scale, the model was verified against wide range of cold-flow data

At equipment scale, the model was verified against plant data

Conclusions

The multiscale CFD model of FCC riser yielded better predictions of cold-flow and reactive flow hydrodynamics.

The EMMS approach was verified using LBM simulations, and it has further potential to be improved.

In general, such multiscale approach should be adopted in simulations of all multiphase reactors.

'Nobody believed the result of a CFD calculation except the one who has generated it.'.....in 1998



'Perhaps today an appropriate statement would be that- Most of the people believe the result except the originator'.....2003

Publications

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- Shah et al., **2013**. Effect of a Cluster on Gas-Solid Drag from Lattice Boltzmann Simulations. **Chemical Engineering Science**, 102, 365-372.
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- Shah et al., **2011**. Hydrodynamics of an FCC riser using energy minimization multiscale drag model. **Chemical Engineering Journal** 168, 812-821.

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Q&A