Recent Advances in CFD Modeling of Multiphase Reactors

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Outline

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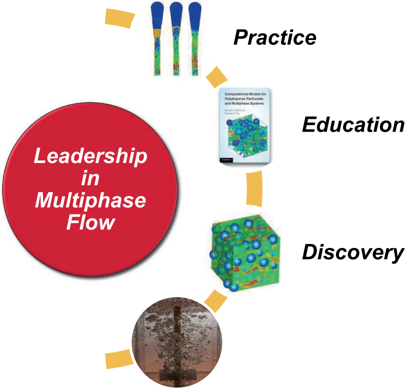
Center for Multiphase Flow Research & Education

Established

- 2014

Vision

- Integrate the activities and expertise of individual research leaders to accelerate knowledge transfer from fundamental scientific advances in multiphase flow to industrial applications.



Research focus

- Multiphase flow research for sustainable production of energy, chemicals, and fuels; manufacture of advanced materials and pharmaceuticals; and development of novel devices and treatments for human health

Annual Research:
~$1.75 million
Funding Sources:
NSF, DOE, ACS, Industry

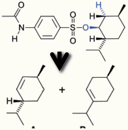
Center for Multiphase Flow Research & Education

Multiphase Reactor Design

LENGTH and TIME SCALES

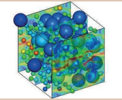
Molecular scale

- Reaction mechanism
- Kinetics
- Solvation effects



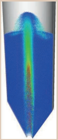
Particle scale

- Flow-chemistry interaction
- Heat-mass transfer
- Interparticle interactions



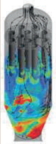
Cluster

- Coupled flow-cluster interaction



Device

- Device performance



System/Plant

- Reduced order models
- Techno-economic analysis

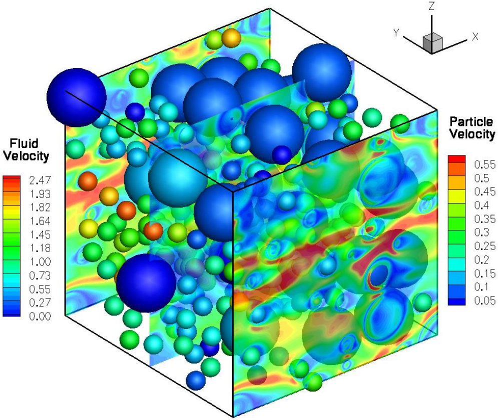
Computational: Subramaniam, Fox, Passalacqua

Experimental: Vigil, Olsen, Heindel

Computational framework for multiphase reactor design to utilize unconventional feed stocks for energy and chemicals

Multiphase Reactors – Modeling Challenges

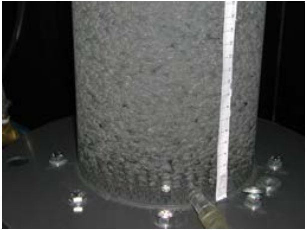
- Continuous phase
- Disperse phase
- Size distribution
- Finite particle inertia
- Particle collisions
- Variable mass loading
- Chemical reactions
- Heat and mass transfer
- Multiphase turbulence



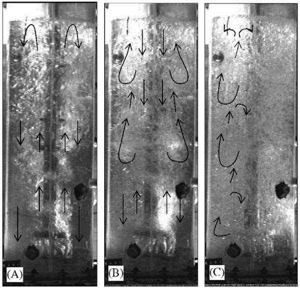
Bidisperse gas–solid flow (DNS of S. Subramaniam)

Multiphase Reactors

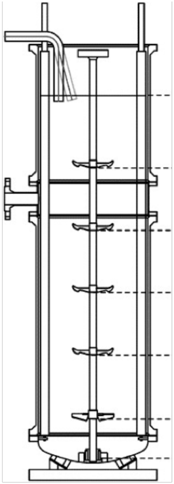
Bubble columns



Gas-liquid reactors

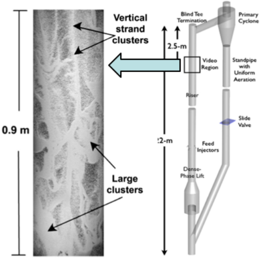


Gas-liquid-solid reactors



Himmelsbach et al., 2006

Gas-solid riser



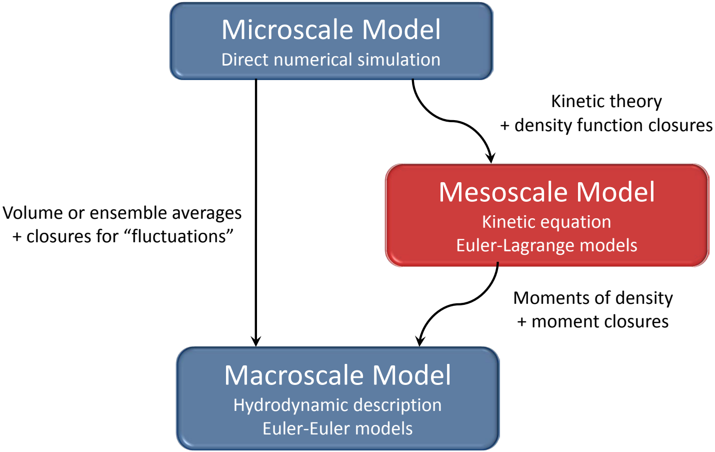
Spray flames

Multiphase Reactors – CFD Modeling Challenges

- Multiphase flows with strong coupling between phases
- Wide range of phase volume fractions (even in same reactor!)
- Inertial particles/droplets with wide range of Stokes numbers
- Polydispersity (e.g. size, density, shape) is always present
- Chemical reactions in one (or all) phases
- Wide range of chemical and physical time scales

Need a robust and versitile CFD modeling framework!

Kinetic-Based Modeling Approach

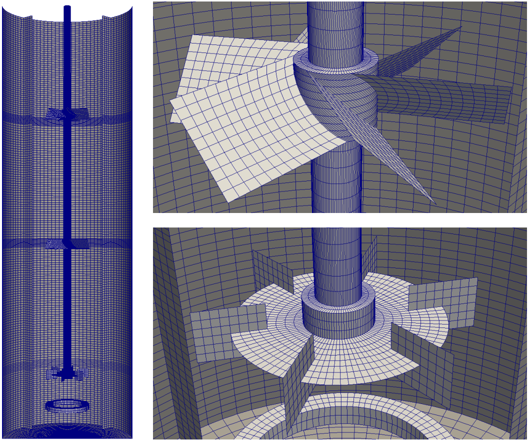


Mesoscale model incorporates more microscale physics in closures!

Multiphase QBMM Framework Based on OpenFOAM

Kinetic-based multiphase models implemented in open-source CFD code

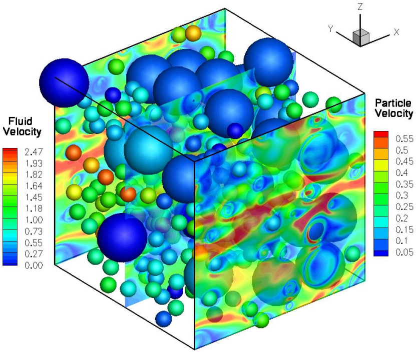
- Consistent and widely adopted framework
- Multi-platform
- Automatic parallelism: industrial-scale computations
- Growing suite of single and multiphase flow models
- Details at www.openqbmm.org



Outline

Gas–Solid Reactors

- solid density $\gg$ gas density
- fluid drag dominants momentum exchange
- particle diameter $\gg 1\ \mu$m
- finite particle inertia (St $\gg$ 1)
- inelastic collisions
- particle size distribution



Kinetic Theory of Granular Flow coupled to gas-phase continuity and momentum balances

Kinetic-Based Model for Gas–Solid Flows

Particle-phase kinetic equation

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{A} n) = \mathbb{C}$$

- $n(t, \mathbf{x}, \mathbf{v})$: velocity NDF
- $\mathbf{v}$: particle velocity
- $\mathbf{A}$: particle acceleration (drag, gravity, ...)
- $\mathbb{C}$: rate of change of n due to particle–particle collisions

Fluid-phase equations

$$\frac{\partial}{\partial t}\left(\rho_g \alpha_g\right) + \nabla \cdot \left(\rho_g \alpha_g \mathbf{U}_g\right) = 0$$

$$\frac{\partial}{\partial t}\left(\rho_g \alpha_g \mathbf{U}_g\right) + \nabla \cdot \left(\rho_g \alpha_g \mathbf{U}_g \mathbf{U}_g\right) = \nabla \cdot \alpha_g \boldsymbol{\tau}_g + \beta_g + \rho_g \alpha_g \mathbf{g}$$

- $\alpha_g = 1 - \alpha_p$: gas volume fraction
- β_g: mean particle drag

Equations coupled through moments of velocity NDF

Lagrangian vs. Eulerian Simulations

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{A} n) = \mathbb{C}$$

Lagrangian method

For large ensemble, particle positions and velocities are tracked

$$\frac{\mathrm{d}\mathbf{x}^{(\alpha)}}{\mathrm{d}t} = \mathbf{v}^{(\alpha)}$$

$$\frac{\mathrm{d}\mathbf{v}^{(\alpha)}}{\mathrm{d}t} = \mathbf{A}^{(\alpha)} + \mathcal{C}^{(\alpha)}$$

Limited by statistical “noise” and coupling errors

Eulerian method

Velocity moments are tracked

$$M^0 = \alpha_\mathrm{p} = \int n \, \mathrm{d}\mathbf{v}$$

$$M_i^1 = \alpha_\mathrm{p} U_{\mathrm{p}i} = \int v_i \, n \, \mathrm{d}\mathbf{v}$$

$$M_{i,j}^2 = \alpha_\mathrm{p} \left(U_{\mathrm{p}i} U_{\mathrm{p}j} + P_{i,j} \right)$$

$$\vdots$$

Moments closed with QBMM

Cluster-Induced Turbulence

Multiphase turbulence generated by momentum coupling

CFD Model for Gas–Solid Flows

Particle phase

$$\frac{\partial}{\partial t}(\rho_p \alpha_p) + \nabla \cdot (\rho_p \alpha_p \mathbf{U}_p) = 0$$

$$\frac{\partial}{\partial t}(\rho_p \alpha_p \mathbf{U}_p) + \nabla \cdot \rho_p \alpha_p (\mathbf{U}_p \mathbf{U}_p + \boldsymbol{\tau}_p) = \rho_p \alpha_p \beta_p + \rho_p \alpha_p \mathbf{g}$$

$$\frac{\partial}{\partial t}(\rho_p \alpha_p \Theta_p) + \nabla \cdot \rho_p \alpha_p (\mathbf{U}_p \Theta_p + \mathbf{q}_p) = -\rho_p \alpha_p \boldsymbol{\tau}_p : \nabla \mathbf{U}_p - \gamma_\Theta$$

Fluid phase

$$\frac{\partial}{\partial t}(\rho_g \alpha_g) + \nabla \cdot (\rho_g \alpha_g \mathbf{U}_g) = 0$$

$$\frac{\partial}{\partial t}(\rho_g \alpha_g \mathbf{U}_g) + \nabla \cdot \rho_g \alpha_g (\mathbf{U}_g \mathbf{U}_g + \boldsymbol{\tau}_g) = -\rho_p \alpha_p \beta_p + \rho_g \alpha_g \mathbf{g}$$

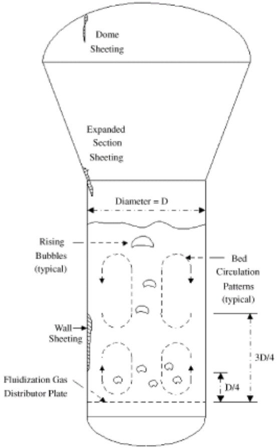
- $\alpha_p + \alpha_g = 1$
- $\beta_p = \frac{1}{\tau_D}(\mathbf{U}_g - \mathbf{U}_p)$
- τ_D: drag time scale
- γ_Θ: granular energy dissipation

Coupled Navier–Stokes Eqs. $\Longrightarrow$ Fluidized-bed reactors

Electrostatics in Fluidized-Bed Reactors

- Chemical, petrochemical, polymer, food, pharmaceutical, agricultural, biochemical industries
- Polyethylene (PE), Polypropylene (PP), Styrenes, Vinyl chloride
- Different grades of PE (LLDPE, LDPE, HDPE)
- Fluidized-bed process
  - Low pressure and temperature
  - Low capital investment and operational costs
  - No solvent separation
  - Excellent heat removal
  - Capability to utilize different catalysts
  - Need to avoid agglomeration and sheeting

Electrostatics in Fluidized-Bed Reactors



Typical locations for fluidized-bed sheeting

G. Hendrickson, CES **61**, 1041–1064 (2006)

Classification of Particles Based on Electrostatic Behavior

- HDPE particles supplied by Univation Technologies
- Particles fluidized at given superficial gas velocity for set time period
- After fluidization period, fluidizing gas is turned off
- Elutriated Particles are collected in filter bag (**FINES**)
- Bed particles dropped into bottom Faraday cup (**DROPPED**)
- Particles stick to wall (**WALL**): thickness and height is measured
- Particle size distribution and charge measurements (**FINES**, **WALL**, **DROPPED**)

R. G. Rokkam et al., CES **92**, 146–156 (2013)

Model for Particle Size Distribution

- Continuity

$$\frac{\partial \rho_{sn}\alpha_{sn}}{\partial t} + \nabla \cdot \rho_{sn}\alpha_{sn}\mathbf{U}_{sn} = 0$$

- Momentum

$$\frac{\partial \rho_{sn}\alpha_{sn}\mathbf{U}_{sn}}{\partial t} + \nabla \cdot \rho_{sn}\alpha_{sn}\mathbf{U}_{sn}\mathbf{U}_{sn} =$$

$$- \alpha_{sn}\nabla p_g - \nabla p_{sn} + \nabla \cdot \boldsymbol{\tau}_{sn} - f_{gn} + \sum_{m=1}^{N} f_{nm} + \rho_{sn}\alpha_{sn}\mathbf{g} + \mathbf{F}_{qsn}$$

ε_{sn}: volume fraction of n^{th} solid phase

$\boldsymbol{\tau}_{sn}$: stress tensor of n^{th} solid phase

$\mathbf{U}_{sn}$: velocity of n^{th} solid phase

$\mathbf{F}_{qsn}$: electrostatic force on n^{th} solid phase

Electrostatic Model

- Gauss law for electric field

$$\nabla \cdot \left[\alpha_{\mathrm{g}} \left(\frac{2.17}{\varepsilon_{\mathrm{g}}} - 1.20 \right) \nabla \varphi \right] = -\frac{1}{\epsilon_0} \sum_{n=1}^{N} q_{\mathrm{s}n} \alpha_{\mathrm{s}n}$$

  - α_{g}, $\alpha_{\mathrm{s}n}$ is gas-phase and n^{th} solid-phase volume fraction
  - φ is electric potential
  - $q_{\mathrm{s}n}$ is n^{th} solid-phase charge

$$\mathbf{F}_{qsn} = -q_{\mathrm{s}n} \alpha_{sn} \nabla \varphi$$

- Electrostatic model coupled with CFD model

Rokkam et al., Powder Technology, **203**, 109-124 (2010)

Algorithm

- Step 1: solve multi-fluid model at every grid point to find α_{g}, $\alpha_{\mathrm{s}n}$
- Step 2: solve Poisson equation

$$\nabla \cdot \left[\alpha_{\mathrm{g}} \left(\frac{2.17}{\alpha_{\mathrm{g}}} - 1.20 \right) \nabla \varphi \right] = -\frac{1}{\epsilon_0} \sum_{n=1}^{N} q_{\mathrm{s}n} \alpha_{\mathrm{s}n}$$

- Step 3: evaluate electrostatic force

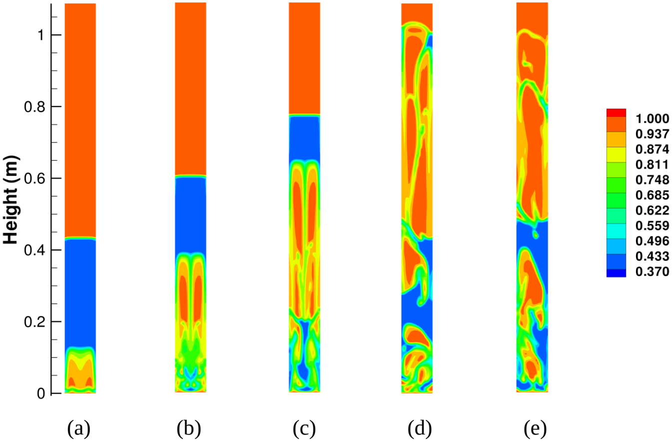
$$\mathbf{F}_{q\mathrm{s}n} = -q_{\mathrm{s}n} \alpha_{\mathrm{s}n} \nabla \varphi$$

- Step 4: add electrostatic force to CFD model in Step 1 and repeat Steps 1, 2, 3, 4 for next iteration

Simulation Parameters

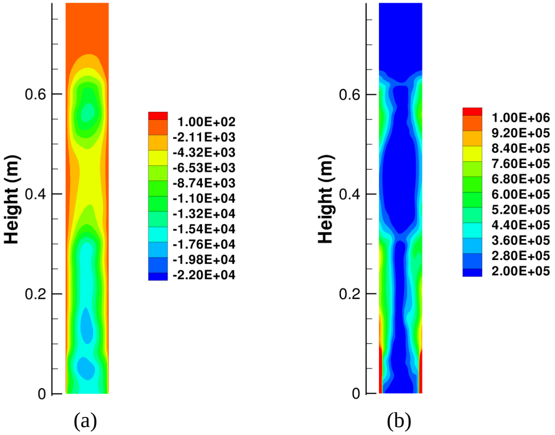
- Cylindrical column
- Eulerian–Eulerian KTGF model for fluidized bed
- Gidaspow drag model for gas–solid interaction
- Electrostatic model as user-defined function
- Gas-phase properties (air)
  - density: 4.93 kg/m^3
  - viscosity: 1.8×10^{-5} kg/(ms)
- Particle-phase properties (HDPE)
  - density: 920 kg/m^3
  - restitution coefficient: 0.8
  - charge distribution q_{sn} measured as function of size

Slug Flow Regime



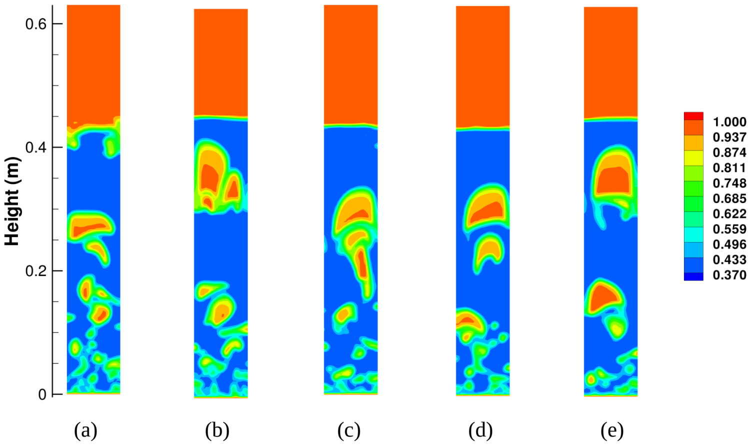
Gas volume fraction (i) 0.22 s (ii) 0.62 s (iii) 1.02 s (iv) 1.62 s (v) 1.82 s

Electric Potential and Electric Field



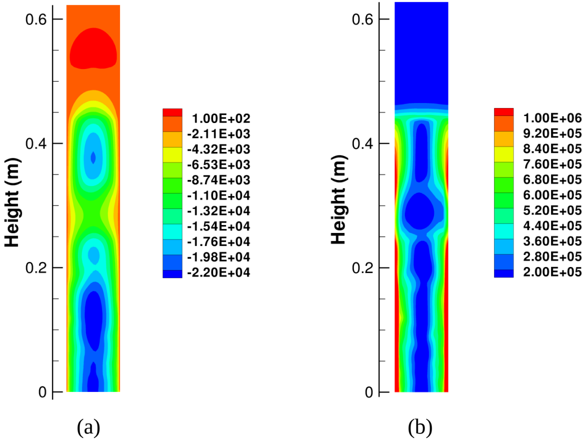
(l) electric potential (V) (r) radial component of electric field (V/m)

Bubbling Flow Regime



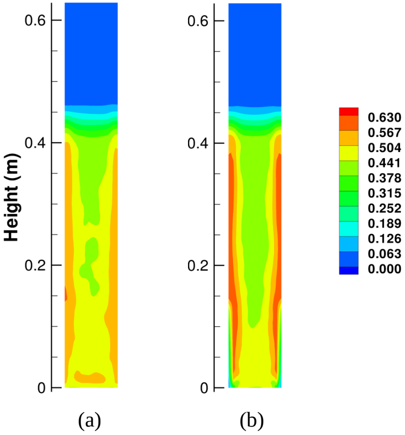
Gas volume fraction (i) 2.30 s (ii) 2.70 s (iii) 3.30 s (iv) 5.50 s (v) 5.70 s

Electric Potential and Electric Field



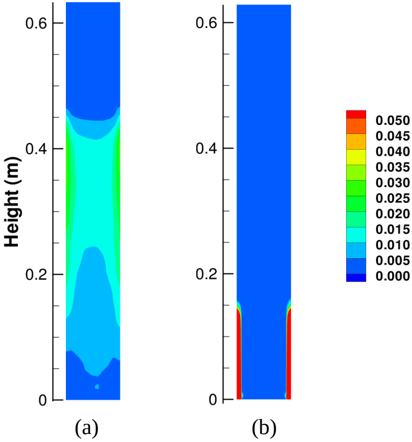
(l) electric potential (V) (r) radial component of electric field (V/m)

Dropped Particles



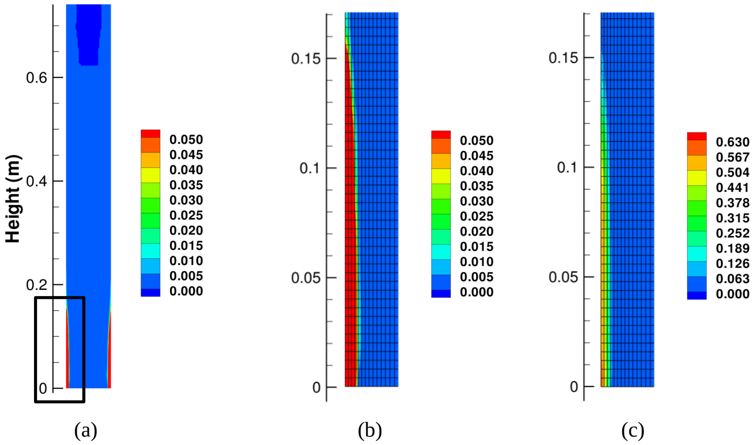
Volume fraction of DROPPED particles (l) no charge (r) charged

Wall Particles



Volume fraction of WALL particles (l) no charge (r) charged

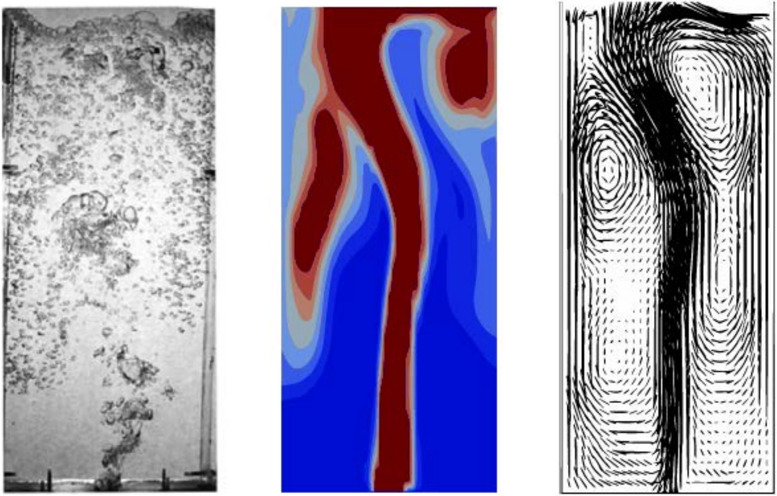
Near Wall Behavior



WALL particles (l) charged (c) zoom (r) different range

Outline

Polydisperse Bubbly Flow



CFD Model for Bubbly Flow

Model must account for

- Liquid-phase continuity and momentum
- Gas-phase continuity and momentum
- Coupling due to buoyancy, drag, virtual mass, lift, wall force, ...
- Bubble size distribution (with size-dependent velocity)
- Coalescence, breakage, mass transfer, ...

Describe bubble phase using **Population Balance Equation**

Generalized Population Balance Equation

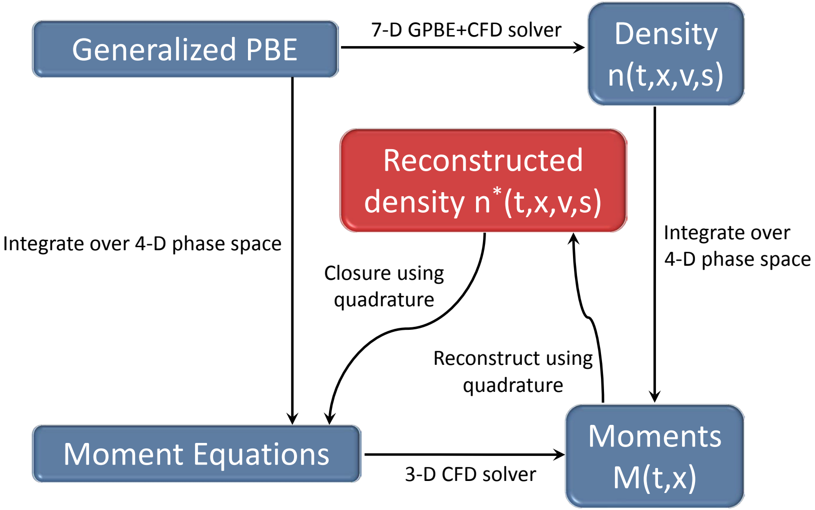
- GPBE has 4-D phase space: bubble velocity $\mathbf{v}$ and bubble size s

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot [\mathbf{A}(t, \mathbf{x}, \mathbf{v}, s)n] + \frac{\partial}{\partial s} [G(t, \mathbf{x}, \mathbf{v}, s)n] = \mathbb{C}$$

  with known acceleration $\mathbf{A}$, growth G and coalescence $\mathbb{C}$ functions

- In principle, a 4-D reconstruction of $n(\mathbf{v}, s)$ is required
- However, bubbles have small inertia relative to liquid
- Use a monokinetic NDF approximation (unique velocity for each size)
- Complex momentum coupling with drag, virtual mass, lift, ...

CFD with Population Balance Equation



Close moment equations by reconstructing density function

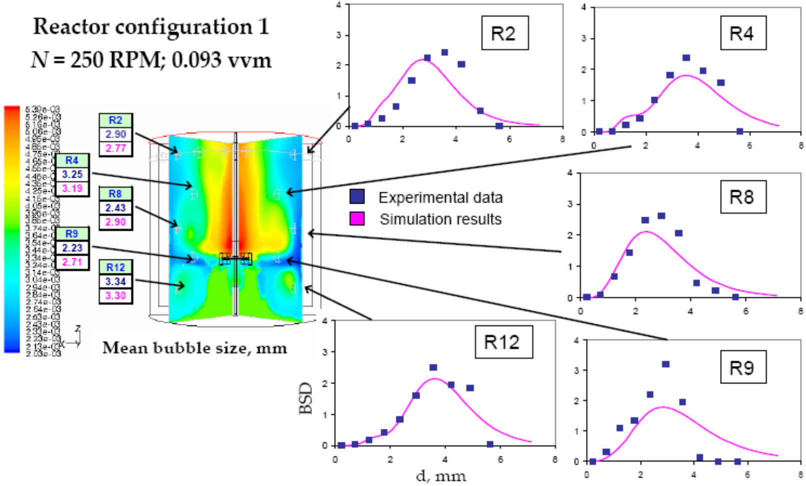
Application to Bubble Column

Volume fraction, bubble-phase velocity, and liquid-phase velocity

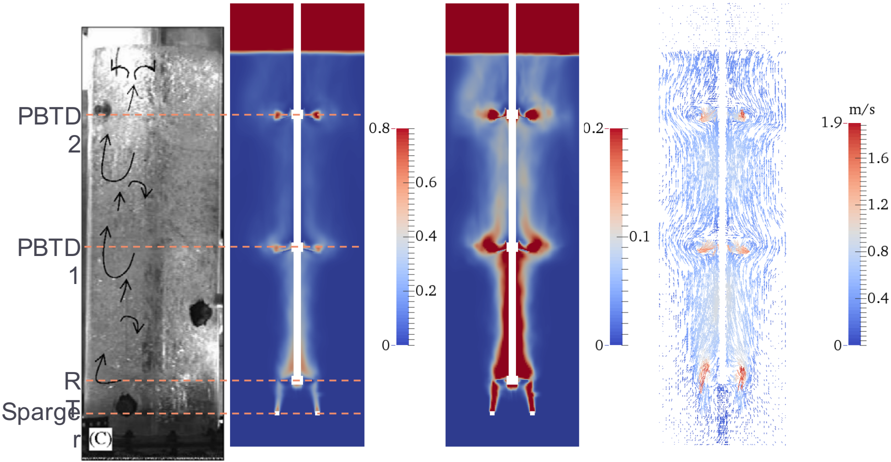
Application to Bubble Column

Volume fraction, mean bubble diameter, and standard deviation

Application to Stirred Reactors



Application to Stirred Reactors



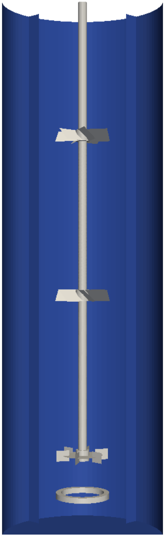
CFD can predict the flow regime as observed in experiments

Summary of CFD Models for Gas–Liquid Reactors

- Generalized PBE includes the velocity of the bubble phase
- Monokinetic NDF approximation valid due to small inertia of bubbles
- Quadrature-Based Moment Methods applied to reconstruct the NDF
- CFD solver modified to treat size-dependent velocity of bubble phase
- Applications to bubble columns and stirred tanks yield good results

Outline

Sparged Slurry Reactor

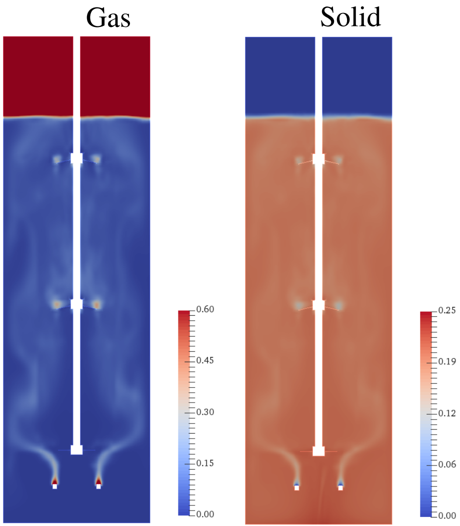


3-fluid CFD model implemented in OpenFOAM:

- Gas phase
  - Monomer with mass transfer to liquid
  - Injected from a sparger
- Liquid phase
  - Solvent containing catalyst
  - Density similar to water
- Solid phase
  - Polymer (growing on catalyst particle)
  - Density slightly larger than water
  - Average particle diameter 150 microns

Interested in solid and gas distribution in reactor and catalyst residence time distribution

Average Phase Distribution at Centerline



- Gas phase
  - Above sparger 10–15%
  - Similar to gas–liquid system
- Solid phase
  - Mostly well mixed: 20%
  - Slightly larger below impellers
  - Does not settle on bottom

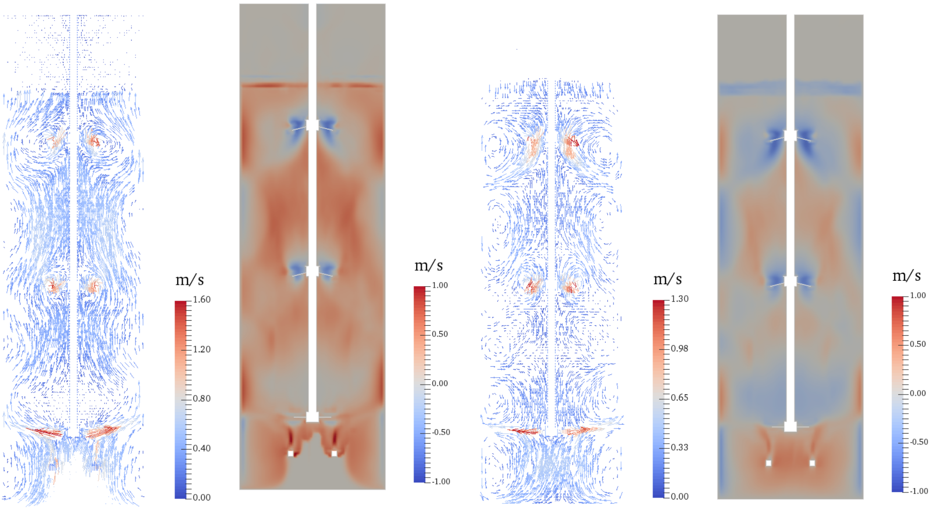
Impellers work as designed
to suspend solids

Average Velocity Distribution at Centerline

Gas: upflow

Liquid (solid):

downflow



Summary of CFD for Gas–Liquid–Solid Reactors

- Gas–liquid flow dominates momentum coupling
- Impeller placement keeps solid phase suspended
- Phase-specific RTD computed in post-processing step
- Complex geometry near impellers requires high-quality mesh
- General flow patterns, power input agree with plant measurements

Outline

Final Remarks

- CFD modeling capabilities have grown enormously in last 25+ years
- Kinetic-based modeling approach uses mesoscale models
- CFD models for multiphase reacting systems solve a Generalized PBE
- Quadrature-based moment methods lead to tractable CFD models
- Simplified electrostatic model for fluidized beds was developed to investigate sheeting
- Predictive multiphase turbulence models are still an open problem
- Efficient and accessible computational framework is now available

Principal Collaborators and Funding Sources

- Gas–Solid Flow: J. Capecelatro, O. Desjardins, B. Kong
- Gas–Liquid Flow: B. Kong, D.L. Marchisio, C. Yuan
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- US National Science Foundation
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