Introduction to Disperse Multiphase Flows

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Examples of Disperse Multiphase Flows

Aerosols

Fine particles

Bubbly/gas–particle flows

Disperse Multiphase Flows with Phase Coupling

- Gas bubbles in liquid phase
  - Bubble columns
  - Bioreactors
  - Boiling heat transfer
- Liquid droplets in gas phase
  - Fuel sprays
  - Irrigation systems
  - Spray coating of pharmaceuticals
- Particles in liquid phase
  - Slurry flow
  - Sedimentation
  - Chemical reactions with solid catalyst
- Particles in gas phase
  - Fluidized-bed reactors
  - Volcanic eruption
  - Carbon capture systems

Computational Fluid Dynamics Modeling

1. Create computational grid
2. Select conservation eqns and closures
   - Mass
   - Chemical species
   - Momentum
   - Energy
   - multiphase, population balance, ...
3. Discretize conservation equations
   - Finite volume for space
   - Stiff ODE solver for reactions
   - Moment method for population balance
   - Lagrangian method for particles, etc.
4. Solve discretized equations
5. Post-process results

Modeling Approach for Disperse Phase

Mesoscale model incorporates more microscale physics in closures!

Examples of CFD Models

- Scalar mixing
  - Reynolds-averaged Navier Stokes (RANS)
  - Composition probability density function (PDF)
  - Large-eddy simulation (LES)
- Reacting flow
  - Flamelet model
  - Look-up table for chemistry
  - Multi-environment PDF model
  - Population balance equation (PBE)
- Polydisperse multiphase flow
  - Generalized population balance equation (GPBE)
  - Kinetic equation for disperse-phase momentum
  - Lagrangian stochastic model for disperse phase

CFD Models for Fine-Particle Formation

Planar jet in a channel: two downstream locations

High Schmidt number in liquid phase

Turbulent Mixing

Confined impinging jets

(c) Re 1500

Transition from laminar to turbulent flow

Turbulent Mixing

Multi-inlet vortex mixer

Complex swirling flow

Models for Scalar Mixing

Choice depends on *Re* and *Sc*

- Laminar flow
  - Direct numerical simulation (DNS)
  - Mixing model for unresolved scales ($Sc \gg 1$)
- Turbulent flow
  - RANS or LES for liquid phase
  - Closures for unresolved scales
- Probability density function (PDF) method
  - PDF transport equation
  - Moments of PDF: mean and variance
  - Closures for transport, mixing

Evolution of PDFs from DNS

Ternary mixing

Binary mixing

- Means are constant $\langle \phi_1 \rangle$ and $\langle \phi_2 \rangle$ (statistically homogeneous)
- Variances decrease: $\langle \phi_1'^2 \rangle$ and $\langle \phi_2'^2 \rangle$
- Simplest CFD model solves for these variables
- Scalar PDF can be fit to moments: β–PDF

CFD Model for Turbulent Mixing

$$\frac{\partial\langle\phi\rangle}{\partial t} + \langle\mathbf{u}\rangle\cdot\nabla\langle\phi\rangle = \nabla\cdot(\Gamma_T\nabla\langle\phi\rangle) \quad \Longrightarrow \quad \text{LSS: large-scale segregation}$$

$$\frac{\partial\langle\phi^2\rangle}{\partial t} + \langle\mathbf{u}\rangle\cdot\nabla\langle\phi^2\rangle = \nabla\cdot(\Gamma_T\nabla\langle\phi^2\rangle) - \varepsilon_\phi \quad \Longrightarrow \quad \text{SSS: small-scale segregation}$$

Confined Impinging-Jets Reactor

Damköhler number

Conversion of undesired product

lines: CFD; symbols: Johnson & Prud'homme (2003)

Large-Eddy Simulation of MIVR

LES

PLIF

LES required to capture strongly swirling flow

LES of MIVR

Bypassing fluid arrives from bottom of mixer

Scale Up of MIVR

Excellent predictions compared to SPIV

Figure 6. Instantaneous velocity field (left: contour plot of velocity magnitude, middle left: vertical crosssection through center of outlet, middle right: horizontal cross-section through center of inlets, right: horizontal cross-section at outlet).

LES predictions are accurate at lab scale and pilot scale

Nanoparticles in Turbulent Mixers

Flash Nanoprecipitation

Produced in CIJR & MIVR

CFD model needed for mixing and population balance

Nanoparticles in Turbulent Flames

Soot

Metal oxides

(Strobel & Pratsinis 2007)

CFD model needed for combustion and population balance

Computational Model for Fine-Particle Formation

Particle size distribution

- Population balance
  - Solve for NDF $n(v)$
  - Coupled to velocity and reactive scalars
  - Non-linear integro-PDE
- Moment methods
  - Solve for moments of NDF
  - Close by reconstructing $n(v)$
  - Quadrature-based moment methods

$$\underbrace{\frac{\partial n(v)}{\partial t}}_{\left(\substack{\text{Rate of}\\ \text{change}}\right)} + \underbrace{\nabla\cdot\left(\mathbf{u}\,n(v)\right)}_{\text{(Convection)}} = \underbrace{\nabla\cdot\left(\Gamma(v,\Phi)\,\nabla n(v)\right)}_{\text{(Particle diffusion)}} + \underbrace{J(\Phi)\,f(v_0)}_{\text{(Nucelation)}}$$
$$+ \underbrace{\int_0^\infty \beta(v-v',v')\,n(v-v')\,n(v')\,dv'}_{\text{(Aggregation-birth)}}$$
$$- \underbrace{\int_0^\infty \beta(v,v')n(v)n(v')\,dv'}_{\text{(Aggregation-death)}} \quad ,$$

Flame Synthesis of Metal–Oxide Particles

- Flamelet model for combustion
- Moment closure for volume–surface NDF $n(v, a)$
- PBE accounts for nucleation, growth, aggregation, and sintering

Large-Eddy-Simulation Results

- m_{10} mean particle volume
- m_{01} mean particle surface area
- N_{pp} primary particles (nuclei)

Main Challenges for CFD with Fine Particles

- Complex flow physics
  - Turbulence in non-canonical geometries
  - Coupling with turbulent mixing and combustion
  - Heat transfer, acoustics, compressible flow
- Complex chemistry
  - Non-equilibrium chemistry (rich, lean)
  - Premixed/nonpremixed/partially premixed combustion
  - Fine particles ('slow' chemistry, high Sc, radiation)
- Fine-particle dynamics
  - Particle size/chemical composition distribution
  - Nucleation, oxidation, surface growth
  - Aggregation, coagulation

Bubbly Flows

Homogeneous

Heterogeneous

Polydisperse Bubbly Flow

Computational Model for Bubbly Flow

Two phases: gas and liquid

- Mass & momentum balances
  - Buoyancy & drag forces
  - Added mass & lift forces
  - Strong phase coupling
  - Flow regime depends on forces

Bubble size distribution (BSD)

- Population balance equation
  - Solve for NDF $n(v)$
  - Size-conditioned bubble velocity
  - Non-linear integro-PDE
- Moment methods
  - Solve for moments of NDF
  - Close by reconstructing $n(v)$

Stirred Reactor with Sparger

Reactor with Bubble Size Distribution

Courtesy of DL Marchisio

Gas–Particle Flows

Volume fraction

Gas velocity

Computational Models for Gas–Particle Flow

Two phases: solid and gas

- Mass, momentum & energy balances from Kinetic Theory of Granular Flow
  - Buoyancy & drag forces
  - Granular temperature
  - Strong phase coupling due to drag

Euler–Euler (EE) & Euler–Lagrange (EL)

- Generalized population balance equation
  - NDF of particle velocity
  - EL solver tracks individual particles
  - EE solver finds moments of NDF
  - Use more moments to capture high Knudsen number flows

Particle Trajectory Crossing

Dilute flow without collisions

Cluster-Induced Turbulence

- Particles fall due to gravity
- Fluid velocity in zero due to pressure gradient
- Clusters form spontaneously
- Clusters drag fluid downward, create wakes
- Fluid turbulence breaks up clusters

Eulerian Versus Lagrangian Models

Cluster-induced turbulence

- Average volume fraction: $\alpha_\mathrm{p} = 0.01$
- $\rho_\mathrm{p}/\rho_\mathrm{g} = 1000$, $\mathrm{Re}_\mathrm{p} = 0.5$
- terminal velocity: $\mathcal{V} = 0.1$ m/s
- cluster length: $\mathcal{L} = 2.5$ mm
- $L_x/\mathcal{L} = 129$ $(2048 \times 512 \times 512)$

Euler–Lagrange and Euler–Euler simulations performed on same grid, but not with same numerical schemes

Qualitative Comparison of Clustering

Case 2 Case 4 Case 6

Similar shapes, but EE has slightly longer/wider clusters

Quantitative Comparison

α_p PDF

Inhomogeneity

Drift velocity

EE has slightly fewer high α_p values (due to numerics?)

EE has slightly higher drift velocity (due to larger clusters?)

Quantitative Comparison of TKE Statistics

Θ_p k_p k_f

EE has lower uncorrelated TKE (due to EL post-processing?)

EE has higher correlated TKE (due to larger clusters?)

Quantitative Comparison of Energy Spectra

α_p U_p U_f

Good agreement at small wavenumbers ($\kappa d_\mathrm{p} < 0.1$)

EE has less energy than EL at large wavenumbers
(due to EL filter for coupling, numerics?)

Particle-Laden Channel Flow

Transition from clusters to bubbles

Effect of Particle Mass Loading

0.2

1.2

20

Bubbling Fluidized Bed

α_p h_2 $U_{p,y}$ Θ_p $\sigma_{p,xy}$

Challenges for CFD of Polydisperse Multiphase Flows

- Complex flow physics
  - Turbulence due to phase coupling
  - Many new unclosed terms in RANS/LES equations
  - Experimental data for flow is largely non-existent
- Lack of scale separation
  - Disperse phase length scale not small
  - Hydrodynamic model difficult to justify
  - Particle-induced versus cluster-induced turbulence
- Disperse-phase dynamics
  - Particle size/chemical-composition/velocity distribution
  - Nucleation, vaporization, dissolution
  - Aggregation, coagulation, coalescence, breakage
  - Drag, buoyancy, lift, virtual mass for momentum exchange

Conclusions

- Computational fluid dynamics can be applied to a wide range of polydisperse multiphase flows
- Multi-scale modeling is required to treat the disparate length and time scales present in most applications
- Development of computational models based on fundamental physics and chemistry is a key step
- Computational methods targeted at accurately solving the computational models are equally important

Successful CFD modeling requires a team effort with complementary skill sets

OpenQBMM Project (www.openqbmm.org)

Polydisperse flow simulation tools in OpenFOAM

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Further Reading

Thanks for your attention!

Questions?