Development of a quadrature-based moment method for polydisperse flows and incorporation in MFIX

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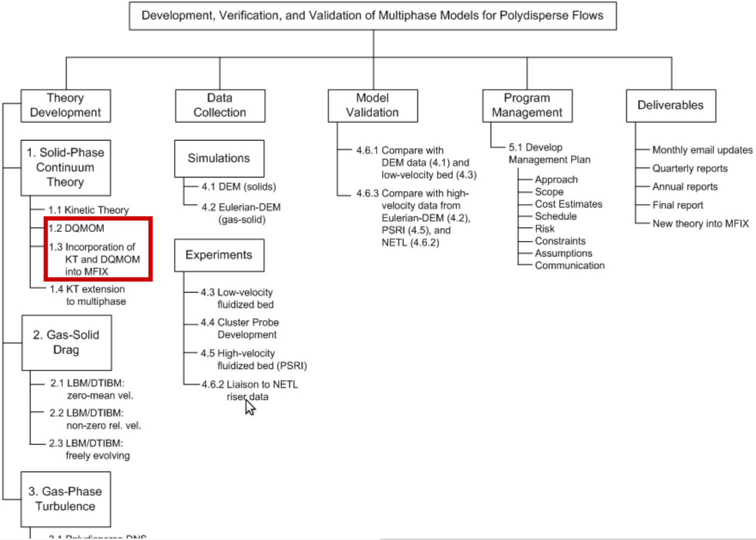
DOE Annual Review Meeting: Development, Verification and Validation of Multiphase Models for Polydisperse Flows
April 22th-23st, 2009 - Morgantown, WV.

Project roadmap



Targeted elements in the roadmap

A1-NT High-fidelity, transient, 3-D, two-phase with PSD (no density variations), hydrodynamics-only simulation of transport reactor.

B6-NT Identify the deficiencies of the current models, assess the state-of-the-art, and document the *current best approach*.

B8-NT Develop a plan for generating validation test cases, identify fundamental experiments, and identify computational challenge problems.

E3-NT Train adequate number of graduate students in this area.

Fundamental equations: Kinetic theory of granular flow

Particle phase kinetic equation

$$\frac{\partial f_i}{\partial t} + \mathbf{v}_i \cdot \frac{\partial f_i}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}_i} \cdot \left(f_i \frac{\mathbf{F}_i}{m_p} \right) = \sum_j \mathbb{C}_{ij}$$

- $f_i\left(\mathbf{v}_i, \mathbf{x}, t\right)$: number density function of species i
- $\mathbf{v}_i$: particle velocity
- $\mathbf{F}_i$: force acting on each particle (drag, gravity, ...)
- $\mathbb{C}_{ij}$: rate of change of f_i due to collisions with species j

Fluid phase equations of motion

$$\frac{\partial}{\partial t}\left(\alpha_\mathrm{f}\rho_\mathrm{f}\right) + \nabla \cdot \left(\alpha_\mathrm{f}\rho_\mathrm{f}\mathbf{U}_\mathrm{f}\right) = 0$$

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- $\beta_{\mathrm{f},i}$: Drag coefficient of species i.

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Characteristic dimensionless parameters

- Fluid phase Reynolds number - How turbulent is the flow?

$$\text{Re} = \frac{\rho_{\text{f}}|\mathbf{U}_{\text{f}}|L}{\mu_{\text{f}}}$$

- Stokes number - How do particles react to the fluid motion?

$$\text{St}_{\text{p}} = \frac{\rho_{\text{p}} d_{\text{p}}^2 |\mathbf{U}_{\text{f}}|}{18\mu_{\text{f}} L}$$

- Mach number - How convective vs. diffusive is the transport?

$$\text{Ma}_{\text{p}} = \frac{|\mathbf{U}_{\text{p}}|}{\Theta^{1/2}}$$

- Knudsen number - How collisional is the particle flow?

$$\text{Ma}_{\text{p}} < 1 \Rightarrow \text{Kn}_{\text{p}} = \sqrt{\frac{\pi}{2}} \frac{\tau_{\text{c}} \Theta^{1/2}}{\text{L}}; \quad \text{Ma}_{\text{p}} > 1 \Rightarrow \text{Kn}_{\text{p}} = \sqrt{\frac{\pi}{2}} \frac{\tau_c |\mathbf{U}_{\text{p}}|}{\text{L}}$$

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Solution methods for the kinetic equation

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Euler-Lagrange method

- The evolution of each particle position and velocity is tracked individually:

$$\frac{\mathrm{d}\mathbf{x}_\alpha}{\mathrm{d}t} = \mathbf{v}_\alpha,$$
$$\frac{\mathrm{d}\mathbf{v}_\alpha}{\mathrm{d}t} = \frac{\mathbf{F}_\alpha}{\mathrm{m_p}}$$

Euler-Euler method

The velocity moments of the distribution function are tracked:

$$M_i^0 = \alpha_{\mathrm{p},i} = \int f_i \mathrm{d}\mathbf{v}_i,$$
$$M_i^1 = \alpha_{\mathrm{p},i}\mathbf{U}_{\mathrm{p},i} = \int \mathbf{v}_i f_i \mathrm{d}\mathbf{v}_i, \ldots$$
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Euler-Euler methods: hydrodynamic vs. moment methods

Hydrodynamic models

- Only low-order moments are tracked: $\alpha_{\mathrm{p},i}$, $\mathbf{U}_{\mathrm{p},i}$, Θ_{p} with Chapman-Enskog expansion to derive constitutive relations
- Expansion valid for $\mathrm{Kn_p} \ll 1$
  - Collision-dominated flows only!
- Two-fluid model + constitutive equations for particle properties

Moment methods

- Moments up to order n are tracked: $\alpha_{\mathrm{p},i}$, $\alpha_{\mathrm{p},i}\mathbf{U}_{\mathrm{p},i}$, $\ldots$, M^n
- Reconstruct velocity distribution function $f(\mathbf{v})$
- Use $f(\mathbf{v})$ to close higher-order moments:
  - Moments spatial fluxes
  - Collision term
  - Force term
- Moment transport equations

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Hydrodynamic models vs. moment methods

Hydrodynamic models

Advantages

- Conceptually simple
- Relatively easy to implement

Disadvantages

- Not valid for $\mathrm{Kn} > 0.1$
- Unable to predict particle trajectory crossing (St_p limitations)
- Difficult to derive physically sound boundary conditions

Moment methods

Advantages

- Valid for arbitrary Knudsen and Stokes numbers
- Can predict particle trajectory crossing
- Easy implementation of *Lagrangian* BCs

Disadvantages

- Computationally inefficient for $\mathrm{Kn} \rightarrow 0$

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Quadrature-based moment method

- The velocity distribution function $f(\mathbf{v})$ is reconstructed using quadrature weights n_α and abscissas $\mathbf{U}_\alpha$:

$$f(\mathbf{v}) = \sum_{\alpha=1}^{\beta} n_\alpha \delta(\mathbf{v} - \mathbf{U}_\alpha)$$

- Quadrature method of moments provides a unique moment-inversion algorithm:

$$\{M^0, M^1, M^2, M^3\} \Leftrightarrow \{n_\alpha, \mathbf{U}_\alpha : \alpha = 1, 2, \ldots, 8\}$$

- The method extends to arbitrary order M^n for increased accuracy

MFIX-QMOM implementation

A new module called MFIX-QMOMB has been added to solve the moment transport equations, fully coupled with the existing fluid solver:

$$\frac{\partial M^0}{\partial t} + \frac{\partial M_i^1}{\partial x_i} = 0$$

$$\frac{\partial M_i^1}{\partial t} + \frac{\partial M_{ij}^2}{\partial x_j} = g_i M^0 + D_i^1$$

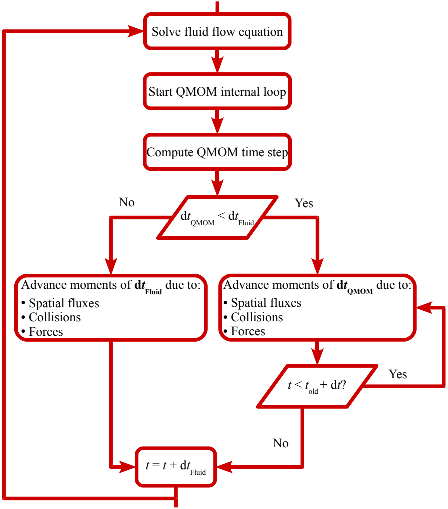
$$\frac{\partial M_{ij}^2}{\partial t} + \frac{\partial M_{ijk}^3}{\partial x_k} = g_i M_j^1 + g_j M_i^1 + C_{ij}^2 + D_{ij}^2$$

$$\frac{\partial M_{ijk}^3}{\partial t} + \frac{\partial M_{ijkl}^4}{\partial x_l} = g_i M_{jk}^2 + g_j M_{ik}^2 + g_k M_{ij}^2 + C_{ijk}^3 + D_{ijk}^3$$

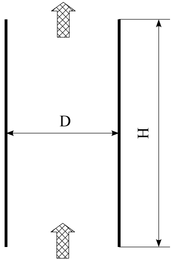
Solution process

QMOM solver:

- Time integration: 2nd order Runge-Kutta scheme
- Space integration: Finite volume method with kinetic flux scheme
- Time split procedure to account for:
    - Spatial fluxes
    - Collisions
    - Forces
- PEA used to couple with fluid solver



Gas-particle flow in a vertical channel



Channel geometry

- $\mathrm{D} = 0.1$ m
- $\mathrm{H} = 1.0$ m

Fluid phase

- $\rho_\mathrm{f} = 1.2$ kg/m^3
- $\mu_\mathrm{f} = 1.73 \cdot 10^{-4}$ Pa s
- $\mathrm{Re} = 1379 < 1500 \Rightarrow$ No turbulence in single-phase flow

Particle phase

- $\overline{\alpha}_\mathrm{p} = 0.04$
- $\rho_\mathrm{p} = 1500$ kg/m^3
- $d_\mathrm{p} = 80, 252.9\ \mu\mathrm{m} \Rightarrow \mathrm{St} = 0.061, 0.61$
- $e = e_w = 1$

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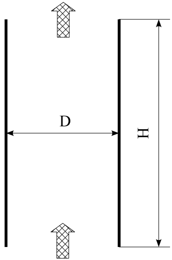

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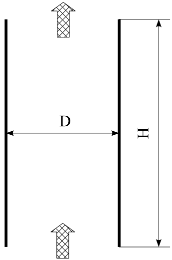

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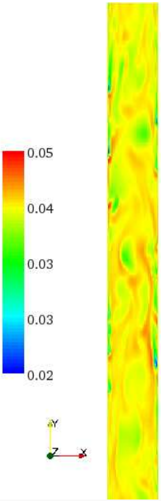
MFIX-QMOM - Two-fluid comparison - St = 0.061

α_p - Two-fluid model



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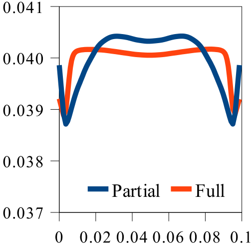

MFIX-QMOM results

- Steady state profiles (no time average!)
- No transient structures

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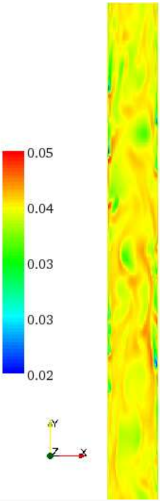

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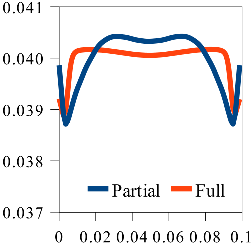

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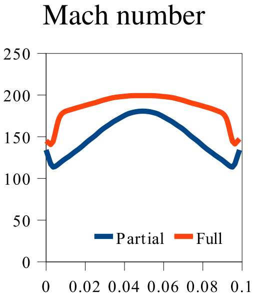

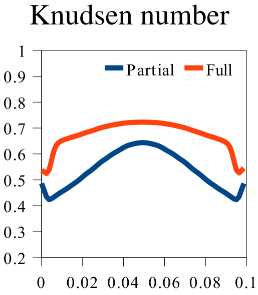

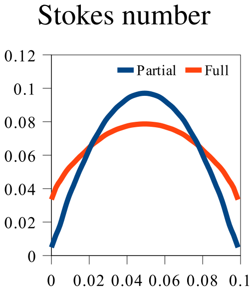

MFIX-QMOM results

- High Mach number flow due to low granular temperature
- $Kn_p > 0.1 \Rightarrow$ Hydrodynamic model + partial slip BCs not valid
- St_p high enough to give particle trajectory crossing

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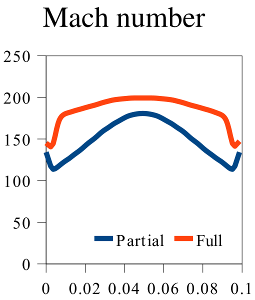

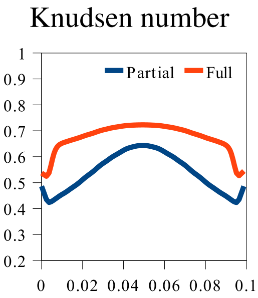

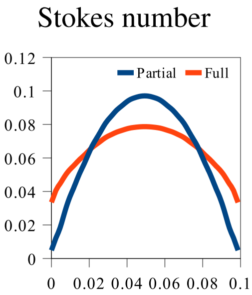

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E-L - Two-fluid comparison: St $= 0.61$

Volume fraction - E-L	Two-fluid model
Loading movie . . .	Loading movie. . .

Mechanism for instability in two-fluid model does not agree with E-L simulations!

E-L - MFIX-QMOM comparison: St $= 0.61$

$\alpha_{\rm p}$ - Euler-Lagrange

QMOM

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Mechanism for instability at finite St is identical in E-L and QMOM.

MFIX-QMOM - Two-fluid comparison: St = 0.61

α_p - Two-fluid model

QMOM

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Quantitative difference between two-fluid and QMOM before/after instability

Conclusions and future work

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Thanks for your attention!