Fully Three-Dimensional Simulations of Riser Flow with a Third-Order Quadrature-Based Moment Method

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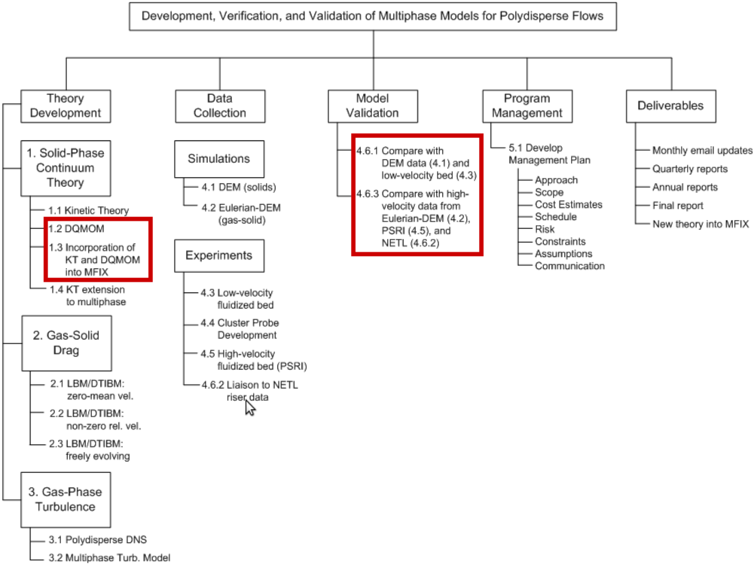
Project roadmap



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*.

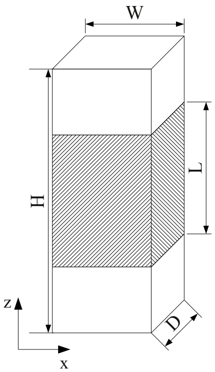
B8-NT Develop a plan for generating validation test cases, identify fundamental experiments, and identify computational challenge problems.

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

Activities during the period 2009 – 2010

- Extension of QMOM to the dense limit: derivation and implementation of moment closures for the Boltzmann-Enskog integral (Fox and Vedula, I&EC Research, 2010)
- Validation of the quadrature method of moments against molecular dynamics data (Passalacqua et al., Comm. Comp. Phys., Under review)
- Two- and three-dimensional verification of the QMOM implementation into MFIX
- Validation of QMOM for gas-particle flows in three-dimensional riser flows (Passalacqua and Fox, ICMF 2010)

Gas-particle flow in a riser



Riser with rectangular section of He et al. (2010)

System properties

- W = 0.05 m
- H = 1.5 m
- D = 0.015 m
- L = 0.30 m

Flow properties

- $d_\mathrm{p} = 335\,\mu\mathrm{m}$
- $\rho_\mathrm{p} = 2500\,\mathrm{kg/m^3}$
- $\rho_\mathrm{f} = 1.2\,\mathrm{kg/m^3}$
- $e_\mathrm{p} = 0.97$
- $G_\mathrm{s} = 10\,\mathrm{kg/(m^3 s)}$
- $U_\mathrm{t} = 2.7\,\mathrm{m/s}$

Fundamental equations: Kinetic theory of granular flow

Particle-phase kinetic equation

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

- $f_i(\mathbf{v}_i, \mathbf{x}, t)$: number density function of species i
- $\mathbf{v}_i$: particle velocity
- $\mathbf{A}_i$: Acceleration 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

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

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_\mathrm{f}\rho_\mathrm{f}\mathbf{U}_\mathrm{f}) &+ \nabla \cdot (\alpha_\mathrm{f}\rho_\mathrm{f}\mathbf{U}_\mathrm{f}\mathbf{U}_\mathrm{f}) \\ &= \nabla \cdot \alpha_\mathrm{f}\boldsymbol{\tau}_\mathrm{f} + \alpha_\mathrm{f}\rho_\mathrm{f}\mathbf{g} \\ &+ \sum_i \beta_{\mathrm{f},i}\left(\mathbf{U}_{\mathrm{p},i} - \mathbf{U}_\mathrm{f}\right) \end{aligned}$$

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

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Quadrature-based moment method for kinetic equations

Moments definition

We define the velocity moments of the distribution function $f_i(\mathbf{v}_i, \mathbf{x}, t)$ as

$$M_i^0 = \alpha_{\mathrm{p},i} = \int f_i \mathrm{d}\mathbf{v}_i,$$

$$M_i^1 = \alpha_{\mathrm{p},i}\mathbf{U}_{\mathrm{p},i} = \int \mathbf{v}_i f_i \mathrm{d}\mathbf{v}_i, \ldots$$

$$M_i^n = \int \mathbf{v}_i^n f_i \mathrm{d}\mathbf{v}_i$$

and obtain moment transport equations by applying their definition to the kinetic equation.

Moment transport equations

We consider a set of twenty moments up to the third-order

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

$$\frac{\partial M_i^1}{\partial t} + \frac{\partial M_{ij}^2}{\partial x_j} = A_i^1$$

$$\frac{\partial M_{ij}^2}{\partial t} + \frac{\partial M_{ijk}^3}{\partial x_k} = A_{ij}^2 + C_{ij}^2$$

$$\frac{\partial M_{ijk}^3}{\partial t} + \frac{\partial M_{ijkl}^4}{\partial x_l} = A_{ijk}^3 + C_{ijk}^3$$

and provide closures (red terms) using quadrature (Fox, 2008).

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Quadrature-based moment method

- 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:

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

- Eight nodes allow the twenty tracked moments to be represented (Fox, 2008)
- Method extends to arbitrary order for increased accuracy (Fox, 2009)

Closures of the moment spatial fluxes

- Spatial fluxes are calculated according to their kinetic formulation:
  - Ensure the realizability of the moments
  - Deal with discontinuous solution fields (shocks) admitted by the moment equations
- For example, for the zero-order moment, we have:

$$\begin{aligned} M_i^1 = Q_i^- + Q_i^+ &= \int_{-\infty}^{0} v_i \left[\int f(\mathbf{v}) dv_j dv_k \right] dv_i + \\ &+ \int_{0}^{+\infty} v_i \left[\int f(\mathbf{v}) dv_j dv_k \right] dv_i \end{aligned}$$

Using the delta function representation of the distribution function, moments components become:

$$Q_i^- = \sum_{\alpha=1}^{\beta} n_\alpha \min\left(0, U_{i,\alpha}\right) \quad Q_i^+ = \sum_{\alpha=1}^{\beta} n_\alpha \max\left(0, U_{i,\alpha}\right)$$

Closures of the acceleration term

- Acceleration term accounts for the effects of
  - Gravity
  - Momentum exchange with the fluid (drag - Wen and Yu (1966))
- Closures are computed as a function of each velocity abscissa (not mean velocity) as

$$A_i^1 = \sum_{\alpha=1}^{\beta} n_\alpha \left(\frac{F_{i\alpha}^{\mathrm{D}}}{m_{\mathrm{p}}} + g_i \right)$$

$$A_{ij}^2 = \sum_{\alpha=1}^{\beta} n_\alpha \left[\left(\frac{F_{i\alpha}^{\mathrm{D}}}{m_{\mathrm{p}}} + g_i \right) U_{j\alpha} + \left(\frac{F_{j\alpha}^{\mathrm{D}}}{m_{\mathrm{p}}} + g_j \right) U_{i\alpha} \right]$$

$$A_{ijk}^3 = \sum_{\alpha=1}^{\beta} n_\alpha \left[\left(\frac{F_{i\alpha}^{\mathrm{D}}}{m_{\mathrm{p}}} + g_i \right) U_{j\alpha} U_{k\alpha} + \left(\frac{F_{j\alpha}^{\mathrm{D}}}{m_{\mathrm{p}}} + g_j \right) U_{k\alpha} U_{i\alpha} + \left(\frac{F_{k\alpha}^{\mathrm{D}}}{m_{\mathrm{p}}} + g_k \right) U_{i\alpha} U_{j\alpha} \right]$$

Closures for the collision term

BGK collision model

Collision term is closed with the BGK collision model, modified to include the effect of the radial distribution function g_0

$$C_{ij}^2 = \frac{\alpha_\mathrm{p}}{\tau_\mathrm{c}} \left(\lambda_{ij} - \sigma_{ij} \right)$$

$$C_{ijk}^3 = \frac{1}{\tau_\mathrm{c}} \left(\Delta_{ijk} - M_{ijk}^3 \right)$$

where the collision time is

$$\tau_\mathrm{c} = \frac{\pi^{1/2} d_\mathrm{p}}{12 \alpha_\mathrm{p} g_0 \Theta_\mathrm{p}^{1/2}}$$

Granular temperature

Granular temperature Θ_p is defined in terms of the moments as

$$\Theta_\mathrm{p} = \frac{1}{3} \left(\sigma_{11} + \sigma_{22} + \sigma_{33} \right)$$

where

$$\sigma_{11} = \frac{M_{11}^2}{M^0} - \left(\frac{M_1^1}{M^0} \right)^2$$

$$\sigma_{22} = \frac{M_{22}^2}{M^0} - \left(\frac{M_2^1}{M^0} \right)^2$$

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Numerical simulation setup

Simulation domain

Central part of the riser is simulated:

- W = 0.05 m
- D = 0.015 m
- L = 0.30 m

Boundary conditions

- Purely reflective walls
- Periodic in the flow direction
- Fixed fluid flow rate to match the solids mass flux

Numerical details

- Grid nodes (WxLxD): 25x60x10 (He et. al. (2010))
- Fluid phase: second order with SuperBee limiter
- Second-order scheme for time integration (adaptive)
- Tolerances: 10^{-4} for all variables at each time step

Data sampling

- Simulation time: 10 s
- Averaging time: 5 s (He et. al. (2010))

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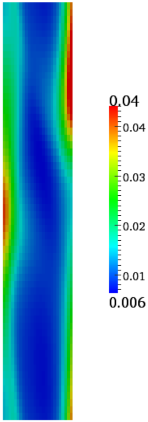
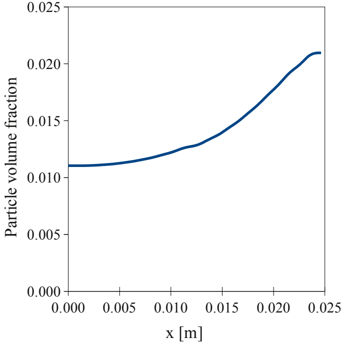
Volume fraction profiles



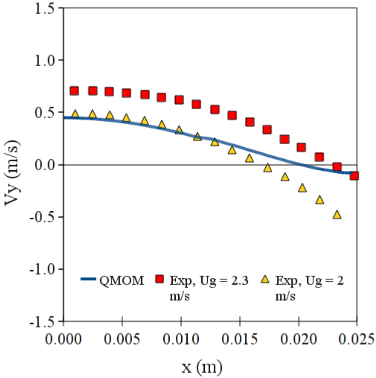
Average volume fraction



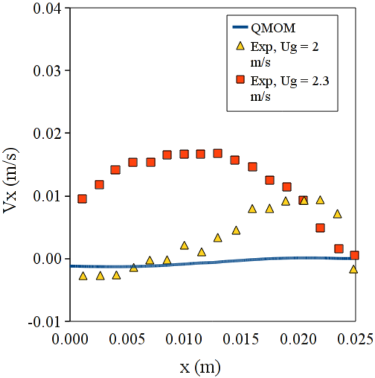
Particle-phase volume fraction at $t = 8$ s

- Core-annular flow structure
- Particle segregation at walls

Averaged velocity components

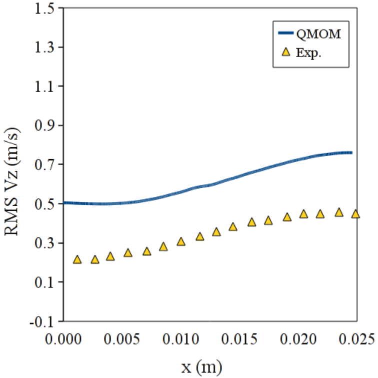


Time averaged *z* (axial) velocity component

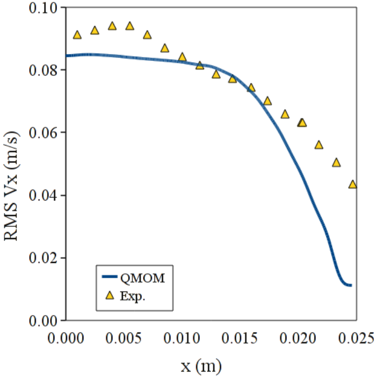


Time averaged *x* velocity component

Averaged velocity components



RMS of the z (axial) velocity component



RMS of x velocity component

Characteristic dimensionless parameters

We examine the dimensionless parameters of the particle phase to better understand the need of higher-order (than hydrodynamic) models:

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

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

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

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

- Knudsen number - How collisional is the particle flow?

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

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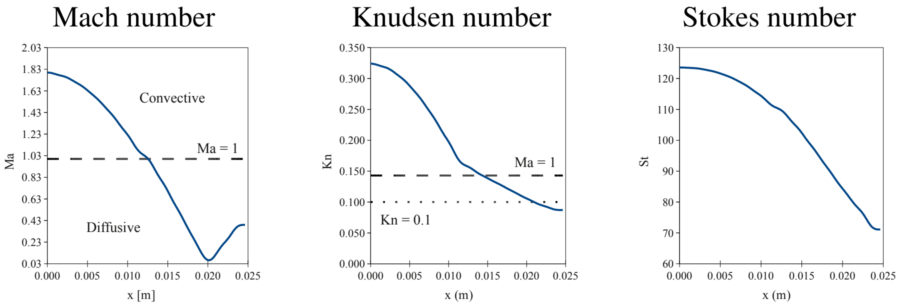
Time-averaged Mach and Knudsen numbers



- Particle flow in transonic conditions ($0.03 < \mathrm{Ma}_p < 1.83$)
- Particle Knudsen number ($0.08 < \mathrm{Kn}_p < 0.32$)
  - always outside the continuum regime ($0.01 < \mathrm{Kn}_p$)
  - slip regime ($0.01 < \mathrm{Kn}_p < 0.1$) only at walls
  - transitional regime ($0.1 < \mathrm{Kn}_p$) in the majority of the system
- High Stokes number ($66.1 < \mathrm{St}_p < 123.5$): particle trajectory crossing

Discussion and conclusions

Examining the dimensionless parameters we found that...

- Flow is not dominated by collisions, but transitions between the slip regime and the transitional regime, where rarefaction effects are not negligible and cannot be dealt with by means of partial-slip boundary conditions
- In most of the riser, flow is dominated by convective phenomena (high Ma), where the hypothesis of equilibrium velocity distribution is not satisfied
- Stokes number is high, making particle-trajectory crossing possible

As a consequence...

Models capable of handling low Ma and high Ma regions, beyond the hydrodynamic limit, with multi-valued local velocities are required to describe riser flows

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Conclusions

- Gas-particle flow in a riser has been simulated using a third-order quadrature-based moment method
- Results for the particle axial velocity and the RMS are in good agreement with the experiments of He et al. (2010), others component are in qualitative agreement with the experiments
- Core-annular flow is captured
- Dimensionless parameters of the system (Ma, St, Kn) are examined, confirming the need of models beyond the hydrodynamic limit, with multi-valued local velocities, to describe riser flows

Future work

- Implementation of Conditional QMOM (CQMOM) to improve the accuracy of the model, keeping the number of quadrature weights fixed (In progress)
- Implementation of dense limit (In progress)
- Validation of the code implementation into MFIX against experimental data in the mono and bi-disperse case

Thanks for your attention!

For Further Reading I

- Fox, R. O., 2008. A quadrature based third-order moment method for dilute gas-particle flows. Journal of Computational Physics 227, 6313 – 6350.
- Fox, R. O., Vedula, P., 2010. Quadrature-based moment model for moderately dense polydisperse gas-particle flows, Industrial & Engineering Chemistry Research, DOI: 10.1021/ie9013138
- He, Y., Deen, N., Van Sing Annaland, M., Kuipers, J. A. M., 2010. Gas-solid turbulent flow in a circulating fluidized bed riser: Experimental and numerical study of monodisperse particle systems, Industrial & Engineering Chemistry Research, 48, 8091 – 8097
- Passalacqua, A., Fox, R. O., Garg, R., Subramaniam, S., 2010. A fully coupled quadrature-based moment method for dilute to moderately dilute fluid-particle flows. Chemical Engineering Science, 65(7):2267 – 2283.