Creating Materials and Energy Solutions

Kinetic Theory Modeling of Turbulent Multiphase Flow

Principal Investigator : Rodney O. Fox

Presenter : Bo Kong

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Project Objectives and Milestones

Objectives :

1. Improve the basic understanding of polydisperse turbulent reacting flows
2. Developing physics-based, mathematically rigorous multiphase flow CFD models
3. Providing input to improve MFiX by widening its applicability

Milestones :

1. FY16Q3 + FY16Q4 : Consistent flux algorithm for size-velocity model for polydisperse particles
2. FY17Q1 : Cutcell technique for complex geometries
3. FY17Q2 : Conditional Hyperbolic Quadrature Method of Moments

Presentation Outline

- Polydisperse Dense Gas-Particle Solver Based on QBMM
  - Background
  - Governing Equations
  - Numerical Method
  - Example Results

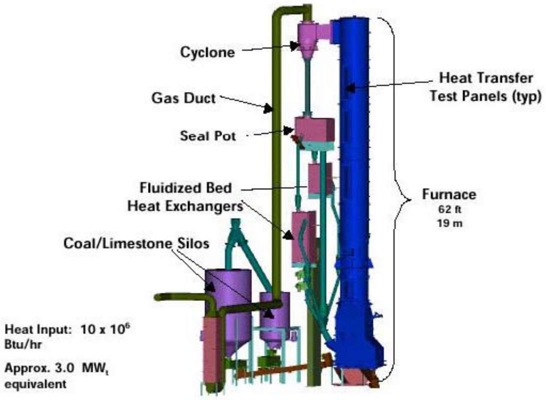
- Conditional hyperbolic quadrature method of moments
  - Example Results

- Summery and Future work

Polydisperse Gas-Particle Solver: Motivation

In many commonly encountered engineering applications:

- Polydispersity (e.g., size, density, shape) is present
- '' Size'' and velocity of disperse phase are closely coupled



Proposed solution: Joint number density function of ``size'' and velocity of disperse phase can be solved using quadrature-based moment methods (QBMM)

Existing models for polydisperse gas-particle flows

Lagrangian methods

- Discrete Element Method (DEM)

  Limitation: Computationally expensive for industrial applications

Eulerian methods

- Population Balance Equation (PBE) carried by fluid velocity

  Limitation: Spatial fluxes do not depend on size

- Class method with separate class velocities

  Limitation: Computationally expensive for continuous size distribution

- Direct Quadrature Method of Moments (DQMOM) with a multi-fluid model

  Limitation: Weights and abscissas are not conserved quantities

Objective :

Develop a robust and accurate moment-based polydisperse flow solver that incorporates microscale physics at reasonable computation cost !!!

Governing Equations : Polydisperse Gas Particle Flows

Gas phase: Continuity and momentum transport equations

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

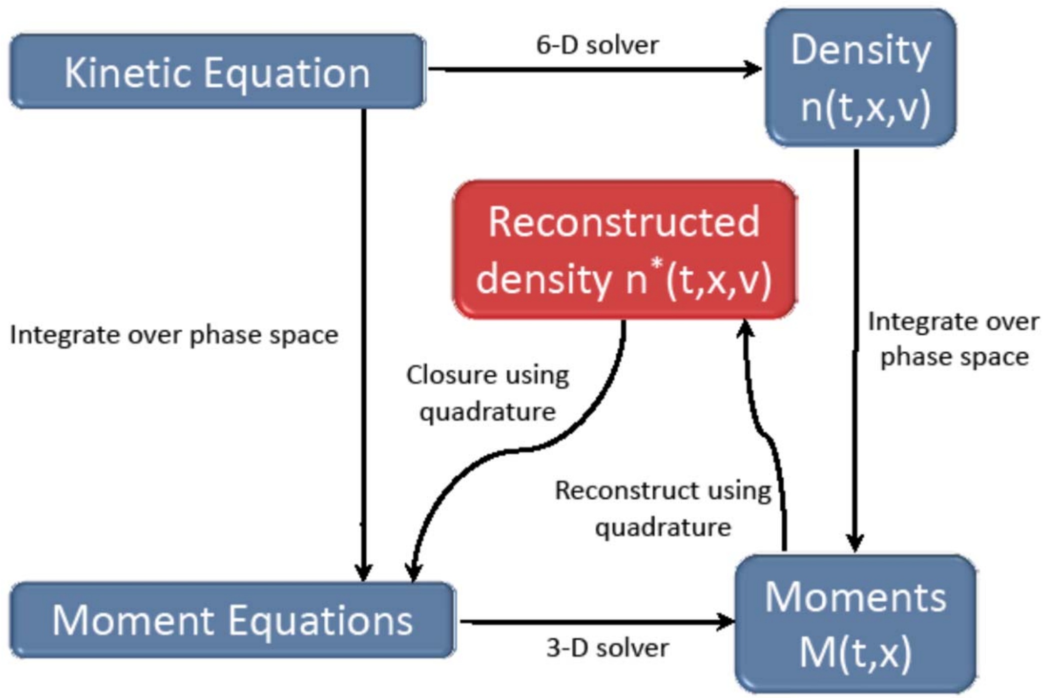
$$\frac{\partial}{\partial t}\rho_g\alpha_g\boldsymbol{U}_g + \nabla\cdot\rho_g\alpha_g\boldsymbol{U}_g\otimes\boldsymbol{U}_g = \nabla\cdot\alpha_g\boldsymbol{\sigma}_g - \alpha_g\nabla p_g + \rho_g\alpha_g\boldsymbol{g} + \boldsymbol{M}_{gp}$$

$$\boldsymbol{M}_{pg} = K_{gp}\left(\boldsymbol{U}_g - \boldsymbol{U}_p\right) - \alpha_p\nabla p_g + \alpha_p\rho_g\nabla\cdot\alpha_g\boldsymbol{\sigma}_g$$

Particle phase: Generalized population balance equation

$$\frac{\partial f(\xi,\boldsymbol{u})}{\partial t} + \boldsymbol{u}\cdot\frac{\partial f(\xi,\boldsymbol{u})}{\partial \boldsymbol{x}} + \frac{\partial}{\partial \boldsymbol{u}}\cdot f(\xi,\boldsymbol{u})\left[\mathbf{A}(\xi,\boldsymbol{u}) + \boldsymbol{g}\right] = \mathbf{C}(\xi,\boldsymbol{u})$$

Solving GPBE with Quadrature-based moments method



Close moment equations by reconstructing density function

Moment sets for solving mas-velocity GPBE

Joint mass-velocity NDF:

$$f(\xi, \boldsymbol{u}) = n(\xi)\, g(\boldsymbol{u} - \boldsymbol{U}(\xi), \Theta(\xi))$$

$$g(\boldsymbol{u} - \boldsymbol{U}(\xi), \Theta(\xi)) = \frac{1}{[2\pi\Theta(\xi)]^{3/2}} \exp\left[-\frac{|\boldsymbol{u} - \boldsymbol{U}(\xi)|^2}{2\Theta(\xi)}\right]$$

Joint mass-velocity moments:

$$M_s := \int_\Omega \xi^s n(\xi) d\xi, \quad \mathcal{U}_s := \int_\Omega \xi^s \boldsymbol{U}(\xi) n(\xi) d\xi, \quad \mathcal{T}_s := \int_\Omega \xi^s \Theta(\xi) n(\xi) d\xi, \quad s \in \mathbb{Z}$$

Moments transport equations

Mass moments:

$$\frac{\partial M_s}{\partial t} + \nabla \cdot \mathcal{U}_s = 0$$

ξ^s-mass-weighted velocity:

$$\frac{\partial \mathcal{U}_s}{\partial t} + \nabla \cdot \left(\mathcal{F}_{u,s} + \mathcal{G}_s + M_s \mathbf{Z}_p\right) = M_s \left(\boldsymbol{g} - \frac{1}{\rho_p} \nabla p_g + \frac{\rho_g}{\rho_p} \nabla \cdot \alpha_g \boldsymbol{\sigma}_g\right) + \mathcal{A}_s + C_s$$

ξ^s- mass-weighted granular temperature:

$$\frac{\partial \mathcal{T}_s}{\partial t} + \nabla \cdot \left(\mathcal{F}_{\Theta,s} + \frac{2}{3} Q_s\right) = -\frac{2}{3} \mathcal{B}_s - \mathcal{A}_{\Theta,s} - C_{\Theta,s}$$

Transport equation for ξ^s-mass-weighted velocity

$$\frac{\partial \mathcal{U}_s}{\partial t} + \nabla \cdot \left(\mathcal{F}_{u,s} + \mathcal{G}_s + M_s \mathbf{Z}_p \right) = M_s \left(\boldsymbol{g} - \frac{1}{\rho_p} \nabla p_g + \frac{\rho_g}{\rho_p} \nabla \cdot \alpha_g \boldsymbol{\sigma}_g \right) + \mathcal{A}_s + C_s$$

Spatial free transport flux:

$$\mathcal{F}_{u,s} = \int_\Omega \xi^s \boldsymbol{U}(\xi) \otimes \boldsymbol{U}(\xi) n(\xi)\, d\xi,$$

Spatial flux due to particle friction:

$$\mathbf{Z}_p = p_{p,f}\mathbf{I} - 2\nu_{p,f}\mathbf{S}_p, \quad p_{p,f} = \frac{Fr}{\rho_p \alpha_p} \frac{\left(\alpha_p - \alpha_{p,fr,min}\right)^{r_1}}{\left(\alpha_{p,max} - \alpha_p\right)^{r_2}} \quad \nu_{p,f} = p_{p,f} \frac{\sin\phi}{\|\mathbf{S}_p\|}$$

Spatial flux due to particle kinetics and collision:

$$\mathcal{G}_s = P_s \mathbf{I} - 2\mu_s \mathbf{S}_s, \quad P_s = \int_\Omega \xi^s p_p(\xi) n(\xi)\, d\xi, \quad \mu_s = \int_\Omega \xi^s \nu_p(\xi) n(\xi)\, d\xi$$

$$p_p(\xi) := \Theta(\xi) + \int_\Omega \frac{2}{3} \eta \alpha(\zeta) g_0(\xi,\zeta) \frac{\chi^3_{\xi,\zeta} \mu_{\xi,\zeta}}{\chi_{\zeta,\xi}} E(\xi,\zeta)\, d\zeta$$

$$\nu_p(\xi) := \frac{d(\xi)\sqrt{\pi\Theta(\xi)}}{12} + \int_\Omega \frac{2}{5} \eta \alpha(\zeta) g_0(\xi,\zeta) \frac{\chi^3_{\xi,\zeta} \mu_{\xi,\zeta}}{\chi_{\zeta,\xi}} \sqrt{E(\xi,\zeta)} \left[d(\xi) + d(\zeta)\right] d\zeta$$

$$E(\xi,\zeta) = 3\Theta(\xi) + 3\Theta(\zeta) + |\boldsymbol{U}(\xi) - \boldsymbol{U}(\zeta)|^2$$

Acceleration source term:

$$\mathcal{A}_s := \int_\Omega \frac{\xi^s}{\tau_p(\xi)} \left[\boldsymbol{U}_g - \boldsymbol{U}(\xi)\right] n(\xi)\, d\xi, \quad \tau_p(\xi) := \frac{4\rho_p d^2(\xi)}{3\rho_g \nu_g C_D(\xi) Re(\xi)}$$

Collisional source term:

$$C_s := \int_\Omega \xi^s C_u(\xi) n(\xi) d\xi, \quad C_u(\xi) := \int_\Omega \frac{\eta}{2\tau_c(\xi,\zeta)} \left[\boldsymbol{U}(\zeta) - \boldsymbol{U}(\xi)\right] \alpha(\zeta)\, d\zeta$$

Transport equation for ξ^s-mass-weighted granular temperature

$$\frac{\partial \mathcal{T}_s}{\partial t} + \nabla \cdot \left(\mathcal{F}_{\Theta,s} + \frac{2}{3} Q_s \right) = -\frac{2}{3} \mathcal{B}_s - \mathcal{A}_{\Theta,s} - C_{\Theta,s}$$

Spatial free transport flux:

$$\mathcal{F}_{\Theta,s} := \int_\Omega \xi^s \boldsymbol{U}(\xi) \Theta(\xi) n(\xi)\, d\xi$$

Granular energy production term:

$$\mathcal{B}_s := \mathcal{G}_s : \nabla \boldsymbol{U}_s,$$

Acceleration source term:

$$\mathcal{A}_{\Theta,s} := \int_\Omega \frac{2\xi^s}{\tau_p(\xi)} \Theta(\xi) n(\xi)\, d\xi.$$

Spatial flux due to particle kinetics and collision:

$$Q_s = -K_s \nabla \Theta_s, \quad K_s = \int_\Omega \xi^s k(\xi) n(\xi)\, d\xi$$

$$k(\xi) := \frac{15 d(\xi) \sqrt{\pi \Theta(\xi)}}{32} + \int_\Omega \frac{3}{5} \eta \alpha(\zeta) g_0(\xi,\zeta) \frac{\chi^3_{\xi,\zeta} \mu_{\xi,\zeta}}{\chi_{\zeta,\xi}} \sqrt{E(\xi,\zeta)} \left[d(\xi) + d(\zeta) \right] d\zeta$$

Collisional source term:

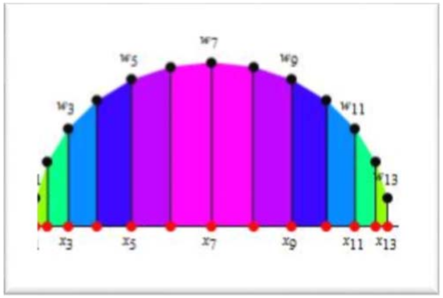
$$C_\Theta(\xi) = S(\xi) - 3J(\xi)\Theta(\xi)$$

$$S(\xi) = \int_\Omega \frac{\eta^2 \mu_{\xi,\zeta}}{4\tau_c(\xi,\zeta)} E(\xi,\zeta) n(\zeta)\, d\zeta, \quad J(\xi) = \int_\Omega \frac{\eta}{2\tau_c(\xi,\zeta)} n(\zeta)\, d\zeta$$

Numerical method: Quadrature-based closure

$$f(\xi, \boldsymbol{u}) = n(\xi)\, g(\boldsymbol{u} - \boldsymbol{U}(\xi), \Theta(\xi))$$

wolfram.com



Mass NDF:

$$n(\xi) = \sum_{\alpha=0}^{N} w_\alpha \delta(\xi - \xi_\alpha),$$

Mass-conditioned velocity and granular temperature:

$$\mathcal{U}_s = \sum_{\alpha=0}^{N} w_\alpha \xi_\alpha^s \boldsymbol{U}_\alpha, \qquad \mathcal{T}_s = \sum_{\alpha=0}^{N} w_\alpha \xi_\alpha^s \Theta_\alpha,$$

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ \xi_0 & \xi_1 & \cdots & \xi_N \\ \vdots & \vdots & \ddots & \vdots \\ \xi_0^N & \xi_1^N & \cdots & \xi_N^N \end{bmatrix} \begin{bmatrix} w_0 & & & \\ & w_1 & & \\ & & \ddots & \\ & & & w_N \end{bmatrix} \begin{bmatrix} \boldsymbol{U}_0 \\ \boldsymbol{U}_1 \\ \vdots \\ \boldsymbol{U}_N \end{bmatrix} = \begin{bmatrix} \mathcal{U}_0 \\ \mathcal{U}_1 \\ \vdots \\ \mathcal{U}_N \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ \xi_0 & \xi_1 & \cdots & \xi_N \\ \vdots & \vdots & \ddots & \vdots \\ \xi_0^N & \xi_1^N & \cdots & \xi_N^N \end{bmatrix} \begin{bmatrix} w_0 & & & \\ & w_1 & & \\ & & \ddots & \\ & & & w_N \end{bmatrix} \begin{bmatrix} \Theta_0 \\ \Theta_1 \\ \vdots \\ \Theta_N \end{bmatrix} = \begin{bmatrix} \mathcal{T}_0 \\ \mathcal{T}_1 \\ \vdots \\ \mathcal{T}_N \end{bmatrix}$$

Solution Algorithm: Separate the Mean and Deviation

Variable decomposition:

$$\boldsymbol{U}_\alpha = \boldsymbol{U}_p + \boldsymbol{V}_\alpha,\ \Theta_\alpha = \Theta_p + \Psi_\alpha$$

$$\mathcal{U}_s = M_s\boldsymbol{U}_p + \mathcal{V}_s, \quad \mathcal{V}_s = \sum_{\alpha=0}^{N} w_\alpha \xi_\alpha^s \boldsymbol{V}_\alpha, \quad \mathcal{T}_s = M_s\Theta_p + \mathcal{W}_s, \quad \mathcal{W}_s = \sum_{\alpha=0}^{N} w_\alpha \xi_\alpha^s \Psi_\alpha$$

"Mean" Transport :

$$\frac{\partial M_1}{\partial t} + \nabla \cdot M_1 \boldsymbol{U}_p = 0$$

$$\frac{\partial M_1 \boldsymbol{U}_p}{\partial t} + \nabla \cdot M_1 \boldsymbol{U}_p \otimes \boldsymbol{U}_p + \nabla \cdot \left(P_1 \mathbf{I} - 2\mu_1 \mathbf{S}_p\right) + \nabla \cdot M_1 \mathbf{Z}_p = M_1 \boldsymbol{g} + K_{gp}\left(\boldsymbol{U}_g - \boldsymbol{U}_p\right) - \frac{M_1}{\rho_p}\nabla p_g + \frac{M_1 \rho_g}{\rho_p}\nabla \cdot \alpha_g \boldsymbol{\sigma}_g$$

$$\frac{\partial M_1 \Theta_p}{\partial t} + \nabla \cdot M_1 \boldsymbol{U}_p \Theta_p - \frac{2}{3}\nabla \cdot K_1 \Theta_p = -\frac{2}{3}\left(P_1 \mathbf{I} - 2\mu_1 \mathbf{S}_p\right) : \nabla \boldsymbol{U}_p - 2K_{gp}\Theta_p + \mathcal{S}_1 - 3\mathcal{J}_1 \Theta_p$$

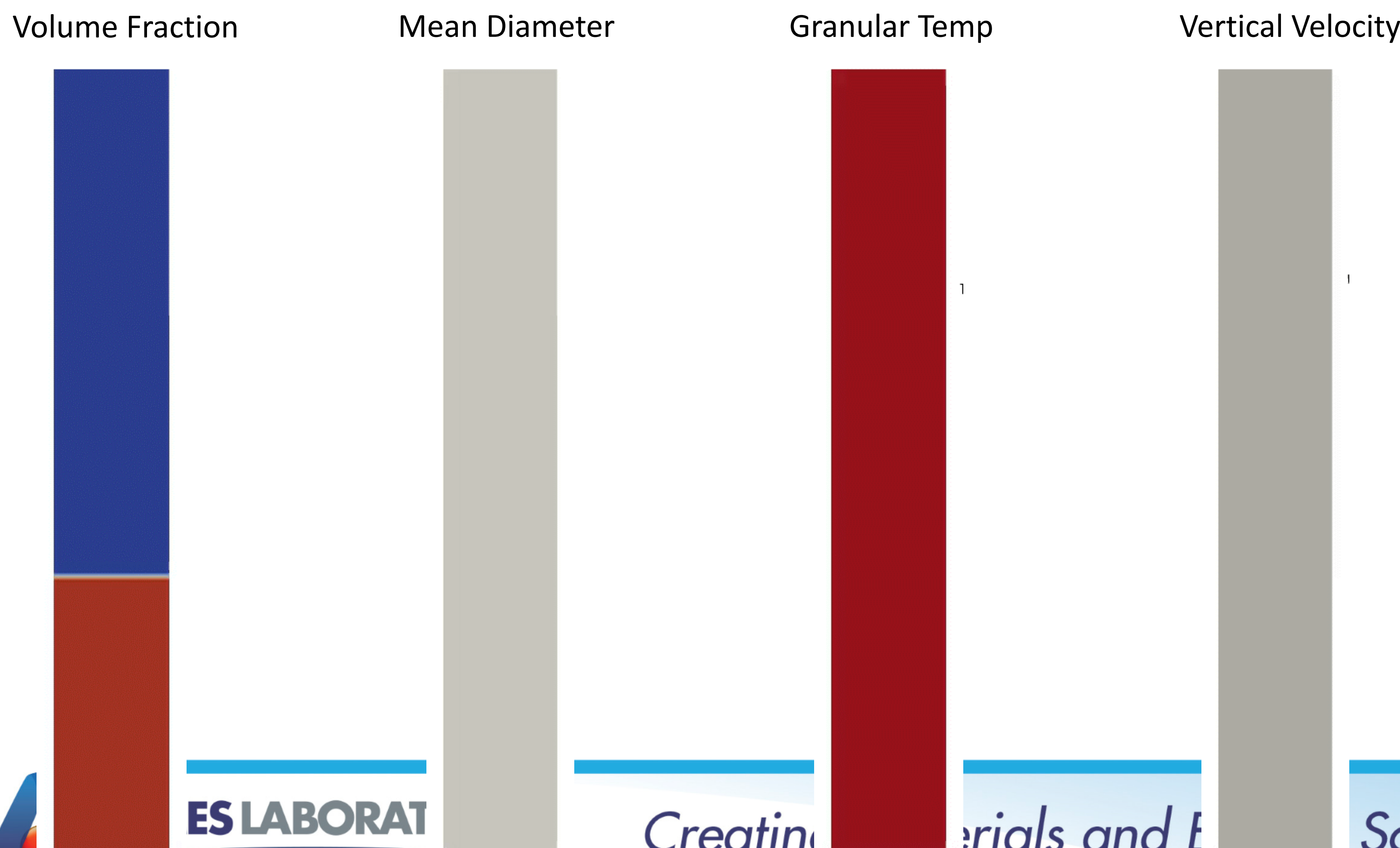
"Deviation" Transport :

$$\frac{\partial M_s}{\partial t} + \nabla \cdot \mathcal{V}_s = 0 \qquad \frac{\partial \mathcal{V}_s}{\partial t} + \nabla \cdot \left(\mathcal{F}'_{u,s} + \mathcal{G}'_s\right) = \mathcal{A}'_s + \mathcal{C}_s \qquad \frac{\partial \mathcal{W}_s}{\partial t} + \nabla \cdot \left(\mathcal{F}'_{\Theta,s} + \frac{2}{3}\mathcal{Q}'_s\right) = -\frac{2}{3}\mathcal{B}'_s - \mathcal{A}'_{\Theta,s} - \mathcal{C}'_{\Theta,s}$$

Overall Solution Algorithm

1. Initialized all variables.
2. Reconstruct mass NDF and conditioned velocity using moment-inversion algorithm.
3. Use a kinetic-based solver to solve particle “Deviation” transport.
4. Reconstruct mass NDF and conditioned velocity again, and calculate parameters used in the “Mean” transport.
5. Use a two-fluid solver to solve particle “Mean” transport and gas phase velocity and pressure fields.
6. Solve for the mass-moment transport new mean velocity and update the mass-weighted velocity and granular temperature.
7. Repeat from step 2 until convergence, and then advance in time.

Example results: polydispersed fluidized bed

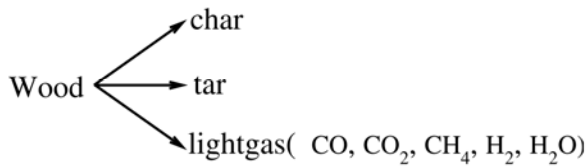


On-going effort

- Particle aggregation and breakage

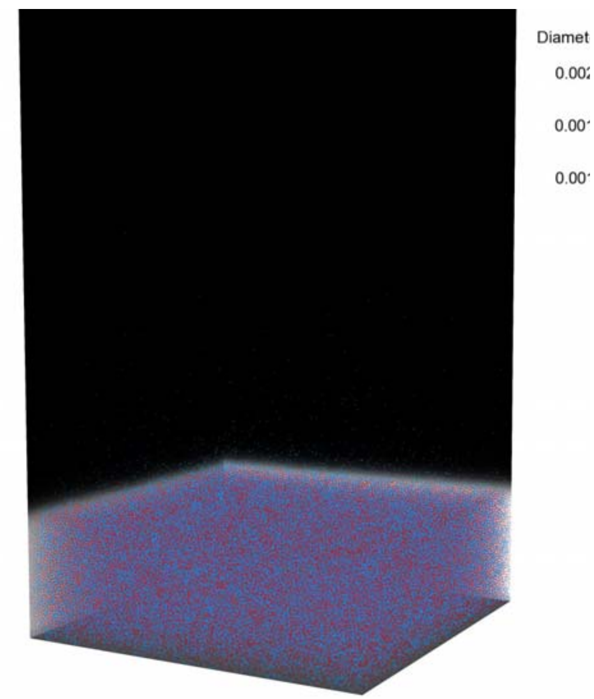
$$\bar{S}_k^{(N)}(\mathbf{x}, t) = \bar{B}_k^a(\mathbf{x}, t) - \bar{D}_k^a(\mathbf{x}, t) + \bar{B}_k^b(\mathbf{x}, t) - \bar{D}_k^b(\mathbf{x}, t),$$

- Chemical reaction -- biomass gasification



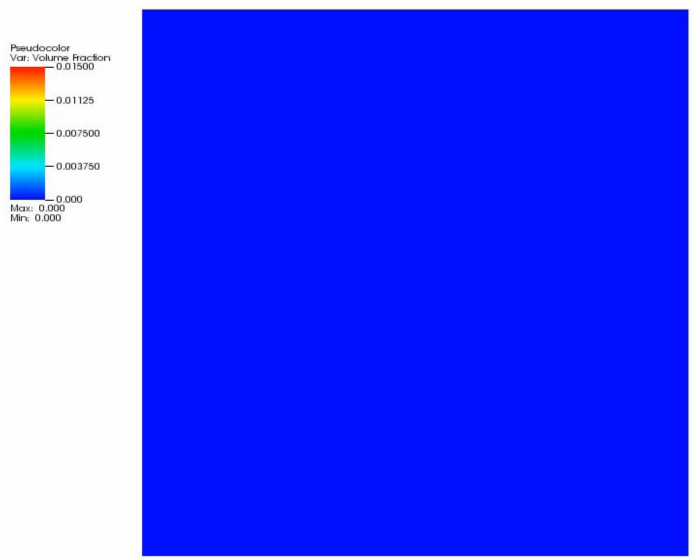
- "Validation" with Goldschmidt et al. (2003) experiments

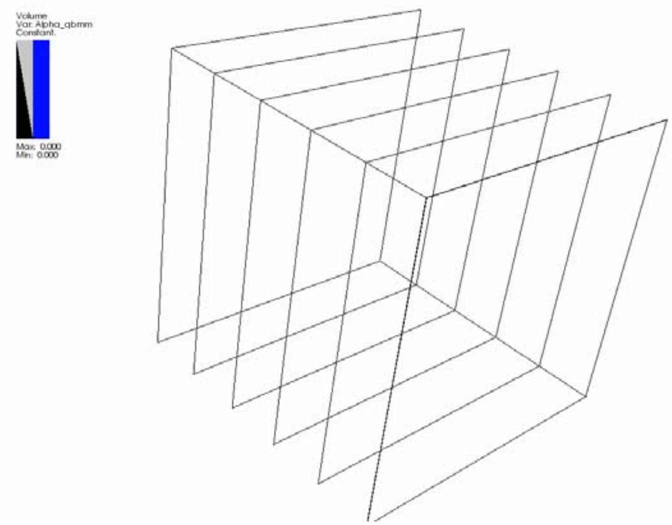
- Perform detailed Euler-Lagrangian simulations to enhance the effective viscosity and conductivity models.



Courtesy of Jesse Capecelatro

Conditional hyperbolic quadrature method of moments (CHyQMOM)





Advantage: Hyperbolic, Smaller moments set, Symmetric, Robust !!!

Summery and Future work

Summery :

1. A new solution algorithm is proposed to solve dense polydispersed gas-particle flows.
2. It was implemented, and then tested in a dense fluidized bed case.
3. It was demonstrated that the new algorithm is computationally robust, and can be used to model various physical and chemical processes.

Milestones :

1. FY17Q3 : Cutcell technique for complex geometries + Implement the already validated new gas-particle turbulence model in MFIX.
2. FY17Q4 : Consolidate previous DQMOM and QMOMK implementation into current MFiX-QBMM module.

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Questions ?