

Extended Conditional Quadrature-Based Moment Methods for Polydisperse Gas-Particle Flows With Size-Conditioned Velocity

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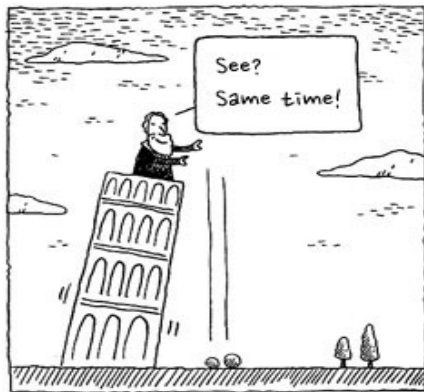
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- 2 Generalized Population Balance Equation (GPBE) and Quadrature Based Moment method (QBMM)
- 3 Extended Quadrature Method of Moments (EQMOM)
- 4 EQMOM with Size-conditioned Velocity
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No, Dear Galileo, you need to buy a new timer!



Topic today: **Size and Velocity !**

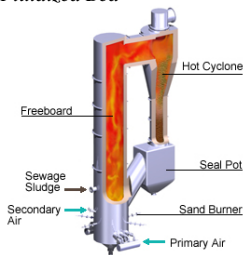
Applications

Polydisperse multiphase flows: continuous phase and **dispersed phase**

Bubble column



Fluidized Bed



Fuel Injection



In all these applications, the size and velocity of the dispersed phase are closely coupled. Thus, to more accurately predict the size distribution of dispersed phase, the joint number density function of particle size and velocity has to be properly modeled.

Generalized Population Balance Equations

Number Density Function : $n(t, \mathbf{x}, \xi, \mathbf{v})$

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i} (v_i n) + \frac{\partial}{\partial v_i} [A_i(t, \mathbf{x}, \xi, \mathbf{v})n] + \frac{\partial}{\partial \xi_j} [G_j(t, \mathbf{x}, \xi, \mathbf{v})n] = \mathbb{C}$$

with acceleration \mathbf{A} , size growth \mathbf{G} and collision/aggregation operator \mathbb{C}

Moment Methods

$$M_{kl} = \int v^k \xi^l n \, dv d\xi$$

Moment Transport Equations

$$\frac{\partial M_{kl}}{\partial t} + \frac{\partial M_{k+1l}}{\partial x} = k \int v^{k-1} \xi^l A n \, dv d\xi + l \int v^k \xi^{l-1} G n \, dv d\xi + \int v^k \xi^l \mathbb{C} \, dv d\xi$$

Terms in red will usually require mathematical closure

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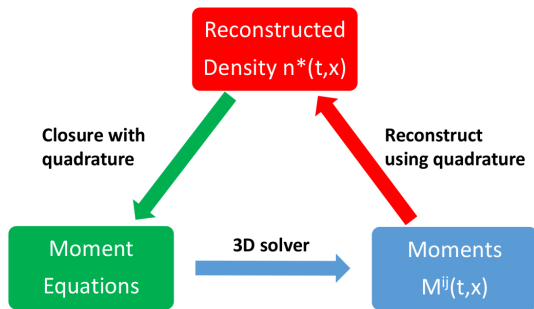
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Quadrature-Based Moment Methods (QBMM)

Close moments equations by reconstructing number density function



The moment-inversion algorithm: $\{M_1, M_2, \dots, M_n\} \Rightarrow n(c_1, c_2, \dots, c_n)$:

- 1 Dirac delta form: traditional Gaussian quadrature, brute-force, tensor product, Conditional quadrature method of moments (CQMOM)
- 2 Continuous function: Extended quadrature method of moments(EQMOM), Extended conditional quadrature method of moments(ECQMOM)

Extended Quadrature Method of Moments (EQMOM)

Extended quadrature method of moments (EQMOM) [Yuan *et al.* (2012)] approximates $f(\xi)$ by sum of kernel density functions:

$$f(\xi) \approx \sum_{\alpha=1}^N w_{\alpha} \delta_{\sigma}(\xi, \xi_{\alpha})$$

with N weights $w_{\alpha} \geq 0$, N abscissas ξ_{α} , but **only one** spread parameter $\sigma \geq 0$, which is determined by fixing one additional moment m_{2N} than traditional QMOM. In the limit $\sigma = 0$, $\delta_{\sigma}(\xi, \xi_{\alpha})$ reduces to Dirac delta function $\delta(\xi - \xi_{\alpha})$.

Advantages of using EQMOM:

- more robust, computationally efficient, and gives a continuous, smooth, non-negative NDF.
- construct a second Gaussian quadrature with respect to kernel density function to achieve higher accuracy.

Kernel density function and example for EQMOM

Kernel density functions

- **Gaussian** ($-\infty < \xi < +\infty$):

$$\delta_\sigma(\xi; \xi_\alpha) \equiv \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\xi - \xi_\alpha)^2}{2\sigma^2}\right)$$

- **Gamma** ($0 < \xi < +\infty$):

$$\delta_\sigma(\xi; \xi_\alpha) \equiv \frac{\xi^{\lambda_\alpha - 1} e^{-\xi/\sigma}}{\Gamma(\lambda_\alpha) \sigma^{\lambda_\alpha}}$$

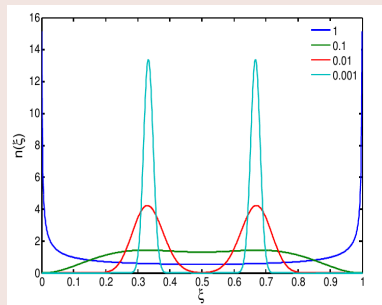
with $\lambda_\alpha = \xi_\alpha/\sigma$.

- **Beta** ($0 < \xi < 1$):

$$\delta_\sigma(\xi; \xi_\alpha) = \frac{\xi^{\lambda_\alpha - 1} (1 - \xi)^{\mu_\alpha - 1}}{B(\lambda_\alpha, \mu_\alpha)}$$

with $\lambda_\alpha = \xi_\alpha/\sigma$ and $\mu_\alpha = (1 - \xi_\alpha)/\sigma$.

Example: 2 nodes beta-EQMOM



$n_1 = n_2 = 1/2, \xi_1 = 1/3, \xi_2 = 2/3$ for different value of σ

First $2N$ moments always exact with max $\sigma : m_{2N} \geq m_{2N}^*(\sigma)$.

Converges to exact NDF as $N \rightarrow \infty$

EQMOM with Size-conditioned Particle Velocity

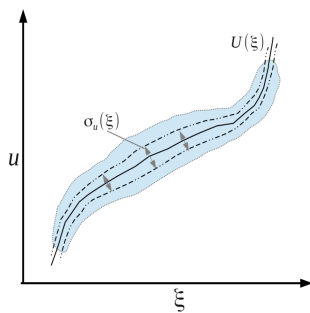
Assuming the velocity distribution for all size is Gaussian, the joint 2-D size-velocity NDF is,

$$f_{s1}(\xi, u) = \sum_{\alpha=1}^{N_s} \rho_{\alpha} K(\xi; \xi_{\alpha}, \sigma_s) g(u - U(\xi); 0, \sigma_u(\xi))$$

$U(\xi)$ and $\sigma_u^2(\xi)$ are size-conditioned velocity mean and variance function. By construction, they are defined to have the following properties:

$$\sum_{\alpha=1}^{N_s} \rho_{\alpha} \int_{\Omega} \xi^i U(\xi) K(\xi; \xi_{\alpha}, \sigma_s) d\xi = M_{i,1} \quad i = 0, \dots, 2N_s$$

$$\sum_{\alpha=1}^{N_s} \rho_{\alpha} \int_{\Omega} \xi^i [U^2(\xi) + \sigma_u^2(\xi)] K(\xi; \xi_{\alpha}, \sigma_s) d\xi = M_{i,2} \quad i = 0, \dots, 2N_s$$



Controlled moments, ($N_s = 2$):

M_{00}	M_{01}	M_{02}
M_{10}	M_{11}	M_{12}
M_{20}	M_{21}	M_{22}
M_{30}	M_{31}	M_{32}
M_{40}	M_{41}	M_{42}

Solve size-conditioned velocity

A natural choice for $U(\xi)$ and $\sigma_u^2(\xi)$ is a sum of orthogonal polynomials,

$$U(\xi) = \sum_{n=0}^{2N_s} a_n p_n(\xi) \quad \sigma_u^2(\xi) = \sum_{n=0}^{2N_s} b_n p_n^2(\xi)$$

p_n is chosen to be shifted Legendre polynomial of order of n for the interval Ω
FOR NOW. a_n and b_n can be determined from a linear system involving a coefficient matrix receptively.

$$\sum_{\alpha=1}^{N_s} \rho_{\alpha} \sum_{n=0}^{2N_s} \langle \xi^i p_n(\xi) \rangle_{\alpha} a_n = M_{i,1} \quad i = 0, \dots, 2N_s$$

$$\sum_{\alpha=1}^{N_s} \rho_{\alpha} \sum_{n=0}^{2N_s} \langle \xi^i p_n^2(\xi) \rangle_{\alpha} b_n = M_{i,1} - \sum_{\alpha=1}^{N_s} \rho_{\alpha} \sum_{n=0}^{2N_s} \sum_{m=0}^{2N_s} \langle \xi^i p_n(\xi) p_m(\xi) \rangle_{\alpha} a_n a_m \quad i = 0, \dots, 2N_s$$

Sample Velocity and its magic

Sample velocity

Second quadrature for Beta kernel function and Gaussian kernel function are,

$$K(\xi; \xi_\alpha, \sigma_s) = \sum_{i=1}^{N_{jq}} \rho_{\alpha i} \delta(\xi, \xi_{\alpha, i})$$

$$g(u; 0, \sigma_u(\xi_{\alpha, i})) = \sum_{j=1}^{N_{hq}} \rho_{\alpha ij} \delta(u, u_{\alpha, i, j})$$

Now, the moments can be calculate as,

$$M_{i,j} = \sum_{\alpha=1}^{N_s} \sum_{i=1}^{N_{jq}} \sum_{j=1}^{N_{hq}} \rho_{\alpha} \rho_{\alpha i} \rho_{\alpha ij} \xi_{\alpha, i}^i \tilde{U}^j$$

where, $\tilde{U} = U(\xi_{\alpha, i}) + u_{\alpha, i, j}$ is the a sample velocity of size $\xi_{\alpha, i}$.

Test case: particle size segregation

General Population Balance Equation:

$$\frac{\partial f}{\partial t} + \frac{\partial v f}{\partial x} + \frac{1}{\tau(\xi)} \frac{\partial v f}{\partial v} = 0$$

where $\tau(\xi) = \tau_0 \xi^{2/3}$ is the characteristic time scale for drag for a particle with normalized size ξ .

Then moment transport equations are

$$\frac{\partial M_{i,j}}{\partial t} + \frac{\partial M_{i,j+1}}{\partial x} = -\frac{j M_{i-2/3,j}}{\tau_0}$$

Using operator splitting method to separate flux terms from drag terms,

$$\frac{\partial M_{i,j}}{\partial t} + \frac{\partial M_{i,j+1}}{\partial x} = 0 \quad ; \quad \frac{\partial M_{i,j}}{\partial t} = -\frac{j M_{i-2/3,j}}{\tau_0}$$

Closure for moment transport equation

Kinetic-based flux

$$F_{x;i,j} = \int_{\mathbb{R}} \left(\int_0^{\infty} f_{s1}(\xi, u) \xi^i u^{j+1} du \right) d\xi + \int_{\mathbb{R}} \left(\int_{-\infty}^0 f_{s1}(\xi, u) \xi^i u^{j+1} du \right) d\xi$$

$$F_{x;i,j} = \sum_{\alpha=1}^{N_s} \sum_{i=1}^{N_{jq}} \sum_{j=1}^{N_{hq}} \rho_{\alpha} \rho_{\alpha i} \rho_{\alpha ij} \xi_{\alpha,i}^i \max(\tilde{U}, 0) + \sum_{\alpha=1}^{N_s} \sum_{i=1}^{N_{jq}} \sum_{j=1}^{N_{hq}} \rho_{\alpha} \rho_{\alpha i} \rho_{\alpha ij} \xi_{\alpha,i}^i \min(\tilde{U}, 0)$$

The realizability condition: $\Delta t = CFL \min_{\alpha,i,j} (\Delta x / |\tilde{U}|)$

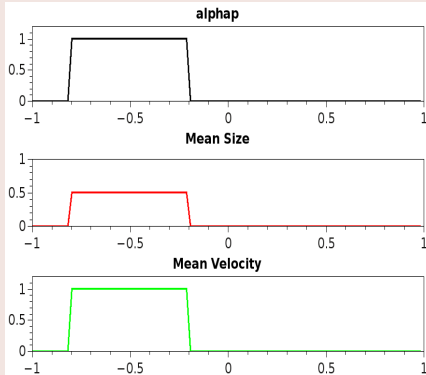
Drag

$$\frac{\partial u}{\partial t} = -\frac{u}{\tau_0 \xi^{2/3}} \quad ; \quad \tilde{U}' = \exp\left(-\frac{\Delta t}{\tau_0 (\xi_{\alpha,i}^i)^{2/3}}\right) \tilde{U} \quad ; \quad M'_{i,j} = \sum_{\alpha=1}^{N_s} \sum_{i=1}^{N_{jq}} \sum_{j=1}^{N_{hq}} \rho_{\alpha} \rho_{\alpha i} \rho_{\alpha ij} \xi_{\alpha,i}^i \tilde{U}'^j$$

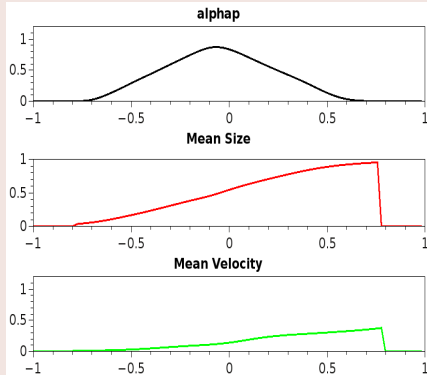
Test case results

At $t = 0$, at $x \in (-0.8, -0.2)$, particle volume fraction $\alpha = 1$, particle size $\xi \in [0, 1]$ has a NDF of unity, and particle velocity has a mean $U = 1$ for all particles.

Initial condition, $t=0$



results, $t = 1$ s



Conclusions and Future Work

- QBMM solves kinetic equation by **reconstructing distribution function from moments**.
- EQMOM reconstruct **continuous, realizable** number density function.
- EQMOM with size-conditioned velocity method can be used to close the MTE effectively.
- More suitable velocity variance function form need to be found.
- This method also need to be extended to 2-D and 3-D cases.

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References I



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