CFD Models for Polydisperse Solids Based on the Direct Quadrature Method of Moments

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Outline

1. **Introduction**
   - **Population Balances**
   - **Coupling with CFD**
2. **Population Balances in CFD**
   - **Population Balance Equation**
   - **Direct Solvers**
   - **Quadrature Methods**
3. **Implementation for Gas-Solid Flow**
   - **Overview of MFIX**
   - **Polydisperse Solids Model**
   - **Application of DQMOM**
4. **Two Open Problems**

Population Balances

- Number density function (NDF)

particle surface area

time

$$n(v, a; x, t)$$

particle volume (mass)

spatial location

CFD provides a description of the dependence of ***n*(*v*,*a*)** on ***x***

For multiphase flows, the NDF will include the phase velocities (as in kinetic theory)

Population Balances

- Moments of number density function

$$m_{kl}(x,t) = \int_0^\infty \int_0^\infty v^k a^l n(v,a;x,t)\,dv\,da$$

Choice of k and l depends on what can be measured

Solving for moments in CFD makes the problem tractable due to smaller number of scalars

Multi-fluid model solves for moments from kinetic theory

Population Balances

- Physical processes leading to size changes
  - Nucleation ➔ ***J(x,t)*** produces new particles, coupled to local solubility, and properties of continuous phase
  - Growth ➔ ***G(x,t)*** mass transfer to surface of existing particles, coupled to local properties of continuous phase
  - Restructuring ➔ particle surface/volume and fractal dimension changes due to shear and/or physio-chemical processes
  - Aggregation/Agglomeration ➔particle-particle interactions, coupled to local shear rate, fluid/particle properties
  - Breakage ➔system dependent, but usually coupled to local shear rate, fluid/particle properties

CFD provides a description of the ***local*** conditions

Population Balances

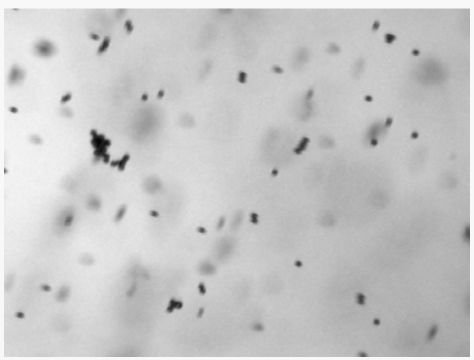
- What can we compare to in-situ experiments?

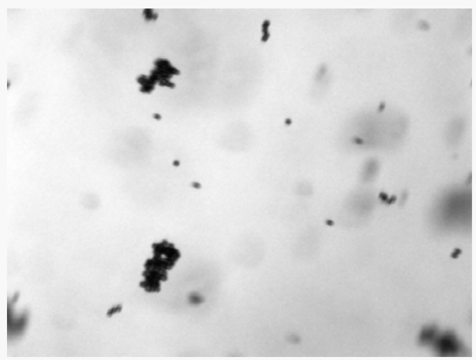
Sub-micron particles ➔ small-angle static light scattering

$$I(0) = C_1 \frac{m_2}{m_1}$$ zero-angle intensity

$$\langle R_g \rangle = C_2 \left(\frac{m_{2(1+d_f)/d_f}}{m_2} \right)^{1/2}$$ radius of gyration $1.8 < d_f < 3$

Larger particles ➔ optical methods





$$n(L),\ L = 2\sqrt{A/\pi}$$ length

$$D_{pf} = 2 \ln(P) / \ln(A)$$

projected fractal dimension

CFD model should predict measurable quantities accurately

Coupling with CFD

- Do particles follow the flow?

  Stokes number

Particle diameter ↓

$$St = \frac{\text{particle response time}}{\text{flow reponse time}} = \frac{\gamma \rho_p d_p^2}{12 \rho_f \nu_f}$$

↑ Kinematic viscosity

If *St* > 0.14, particle velocities must be found from a separate momentum equation in the CFD simulation

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Coupling with CFD

- Do PBE timescales overlap with flow timescales ?

Residence time $\tau = V/q$

Recirculation time $t_c \propto D_T/(N_I D_I)$ or D_T/U_j

Local mixing timescale $t_u = k/\langle\epsilon\rangle$

Kolmogorov timescale $t_\eta = (\nu/\langle\epsilon\rangle)^{1/2}$

CFD simulations w/o PBE can be used to determine timescales for a particular piece of equipment

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Population Balance Equation

- Typical NDF Transport Equation (small Stokes)

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i}(U_i n) = \quad \text{Advection}$$

$$\frac{\partial}{\partial x_i}\left(D_T \frac{\partial n}{\partial x_i}\right) \quad \text{Diffusion}$$

$$+ J(v) - \frac{\partial}{\partial v}(G(v)n) \quad \text{Nucleation + Growth}$$

$$\left.\begin{aligned} &+ \frac{1}{2}\int_0^v \beta(v-s,s)n(v-s)n(s)ds \\ &- n(v)\int_0^\infty \beta(v,s)n(s)ds \end{aligned}\right\} \text{Aggregation}$$

$$+ \int_v^\infty b(v|s)a(s)n(s)ds - a(v)n(v) \quad \text{Breakage}$$

Population Balance Equation

- Aggregation Kernel

$$\beta(v,s) = \frac{2K_BT}{3\mu W}\left(v^{1/d_f} + s^{1/d_f}\right)\left(v^{-1/d_f} + s^{-1/d_f}\right) \quad \text{Brownian}$$

$$+\gamma\alpha(v,s)v_p\left(v^{1/d_f} + s^{1/d_f}\right)^3 \quad \text{Shear-induced}$$

Sub-micron aggregates: Brownian >> Shear-induced

Breakage and restructuring determine fractal dimension d_f

In granular flow, particle-particle collisions must be added

Population Balance Equation

- Breakage Kernels

$$a(v) = c\gamma \exp\left(-\frac{B(\gamma)}{\gamma^2 R_p v^{1/d_f}}\right)$$ exponential

$$a(v) = c_1 \gamma^{c_2} \left(R_p v^{1/d_f}\right)^{c_3}$$ power law

Breakage due to fluid shear only ==> additional term due to collisions in gas-solid flows

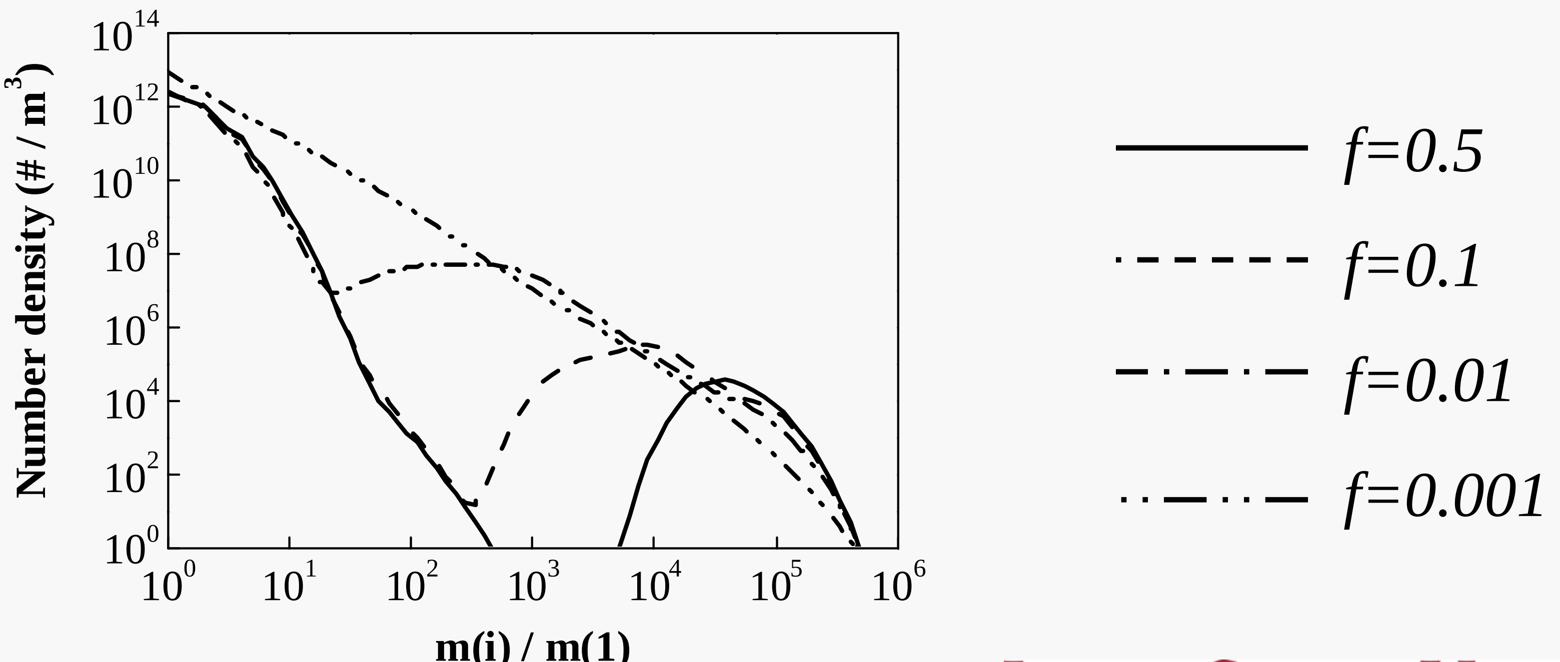
Parameters determined empirically and depend on chemical/physical properties of aggregates

Population Balance Equation

- Daughter Distribution

$$b(v|s) = \delta\left(v - fs\right) + \delta\left(v - (1 - f)s\right)$$ binary

Equal sized: $f = ½$ Erosion: $f << 1$



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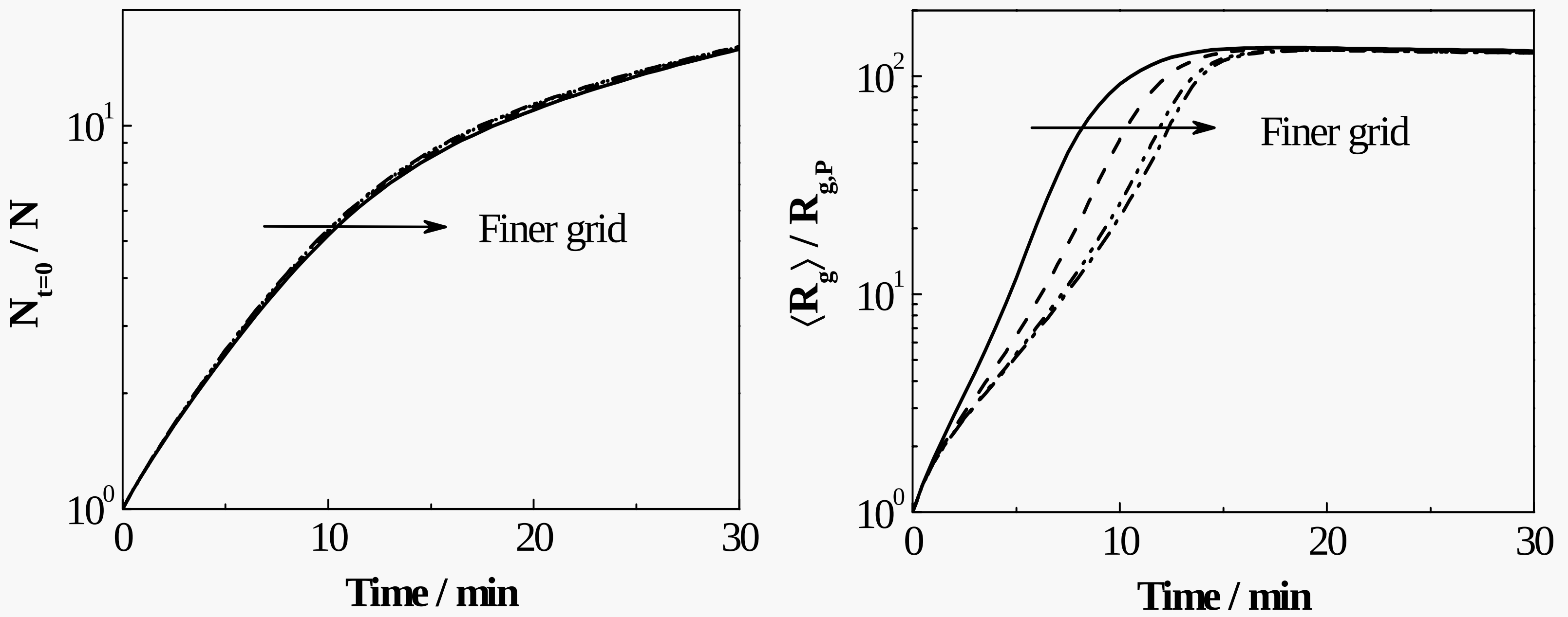
Direct Solvers

- Sectional or Class Methods



Accurate predictions for higher-order moments require finer grid (range: 25-120 bins)

Direct Solvers

- Difficulties encountered when coupled with CFD
  - $n(v; x, t)$ represented by N scalars $n_i(x,t)$ where $25<N<120$
  - Depending on kernels, initial conditions, etc., source terms for these scalars can be stiff
  - If particles are large (measured by Stokes number), multiphase models with N momentum equations required
  - Extension to multi-variate distributions scales like N^D – accounting for "morphology" changes will be intractable

Need methods that accurately predict experimentally observable moments, but at low computational cost

Quadrature Methods

- Quadrature Method of Moments (QMOM)

weights abscissas

$$n(v;x,t) \approx \sum_{n=1}^{N} w_n \delta(v - v_n)$$

*k*th moment of CSD:

$$m_k = \sum_{n=1}^{N} w_n v_n^k$$

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Quadrature Methods

- Product-Difference algorithm (univariate CSD)

$$\{m_0, m_1, m_2, m_3, m_4, m_5, m_6, m_7\}$$

$$\downarrow$$

$$\{w_1, w_2, w_3, w_4, v_1, v_2, v_3, v_4\}$$

Inverse problem solved on the fly in CFD simulation

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Quadrature Methods

- Transport $2N$ moments in CFD simulation

$$\frac{\partial m_k}{\partial t} + \frac{\partial}{\partial x_i}(U_i m_k) =$$ Advection

$$\frac{\partial}{\partial x_i}\left(D_T \frac{\partial m_k}{\partial x_i}\right)$$ Diffusion

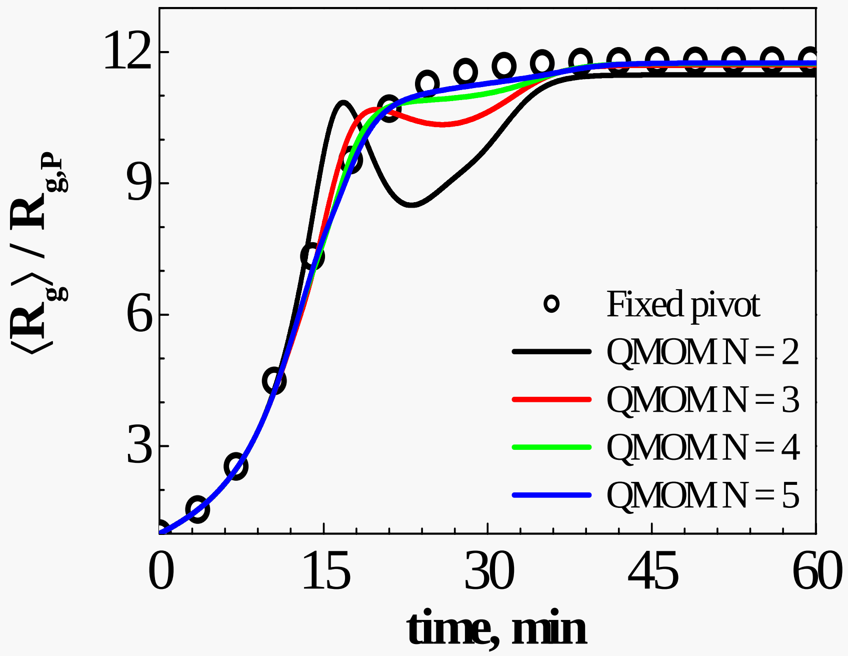
$$+ J_k + \sum_i k v_i^{k-1} G_i w_i$$ Nucleation + Growth

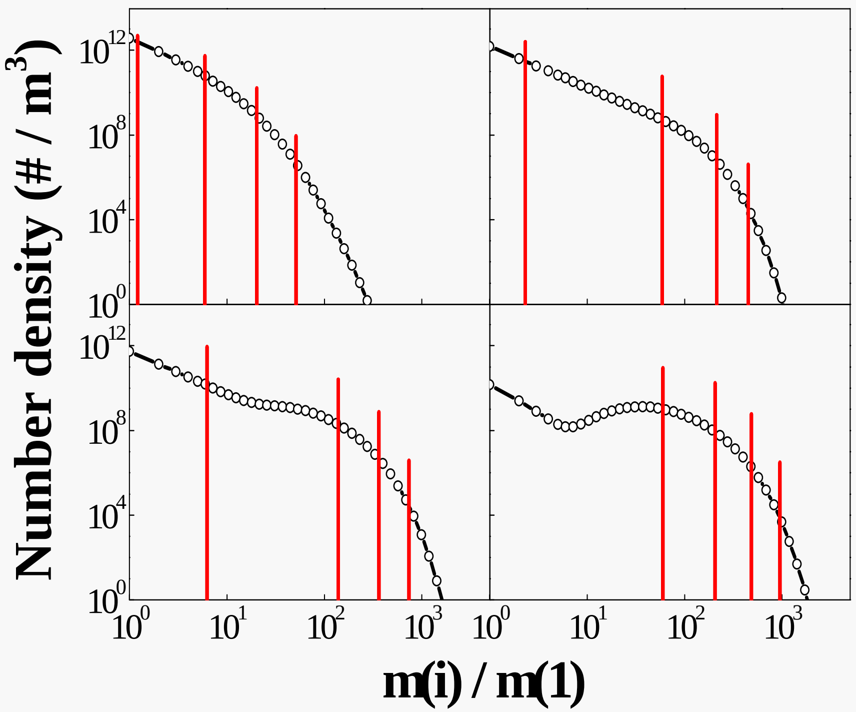
$$+ \frac{1}{2}\sum_i \sum_j \left[(v_i + v_j)^k - v_i^k - v_j^k\right] \beta_{ij} w_i w_j$$ Aggregation

$$+ \sum_i a_i \left[b_i^{(k)} - v_i^k\right] w_i$$ Breakage

Quadrature Methods

- Comparison with direct method





Using $2N = 8$ scalars, QMOM reproduces the grid-independent moments of the direct method

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Quadrature Methods

- Multi-variate extension is straightforward

weights abscissas

$$n(v,a;x,t) \approx \sum_{n=1}^{N} w_n \delta(v - v_n)\delta(a - a_n)$$

(*k*,*l*)th moment of CSD:

$$m_{kl} = \sum_{n=1}^{N} w_n v_n^k a_n^l$$

But inverse problem cannot be solved on the fly!

Quadrature Methods

- Direct Quadrature Method of Moments (DQMOM)

$$\frac{\partial w_n}{\partial t} + \frac{\partial}{\partial x_i}(U_i w_n) = \frac{\partial}{\partial x_i}\left(D_T \frac{\partial w_n}{\partial x_i}\right) + \alpha_n$$ Weights

$$\frac{\partial w_n v_n}{\partial t} + \frac{\partial}{\partial x_i}(U_i w_n v_n) = \frac{\partial}{\partial x_i}\left(D_T \frac{\partial w_n v_n}{\partial x_i}\right) + \alpha_{1n}$$ Volume

$$\frac{\partial w_n a_n}{\partial t} + \frac{\partial}{\partial x_i}(U_i w_n a_n) = \frac{\partial}{\partial x_i}\left(D_T \frac{\partial w_n a_n}{\partial x_i}\right) + \alpha_{2n}$$ Area

Source terms found from linear system on the fly

$$\sum_{n=1}^{N}(1-k)\phi_n^k \alpha_n + \sum_{n=1}^{N} k\phi_n^{k-1}(c_v \alpha_{1n} + c_a \alpha_{2n}) = R_k$$

$$\phi_n = c_v v_n + c_a a_n$$

Polydisperse Gas-Solid Flow

- DQMOM with size and momentum of solid phase

$$\frac{\partial w_\alpha}{\partial t} + \nabla \cdot (\mathbf{U}_\alpha w_\alpha) = a_\alpha$$ Number

$$\frac{\partial \rho w_\alpha v_\alpha}{\partial t} + \nabla \cdot (\mathbf{U}_\alpha \rho w_\alpha v_\alpha) = \rho b_\alpha$$ Mass

$$\frac{\partial \rho w_\alpha v_\alpha \mathbf{U}_\alpha}{\partial t} + \nabla \cdot (\rho w_\alpha v_\alpha \mathbf{U}_\alpha \mathbf{U}_\alpha) = \rho \mathbf{c}_\alpha$$ Momentum

Source terms for mass and momentum can be found from kinetic theory for gas-solid flows

Reduces to two-fluid model when $\alpha=1$

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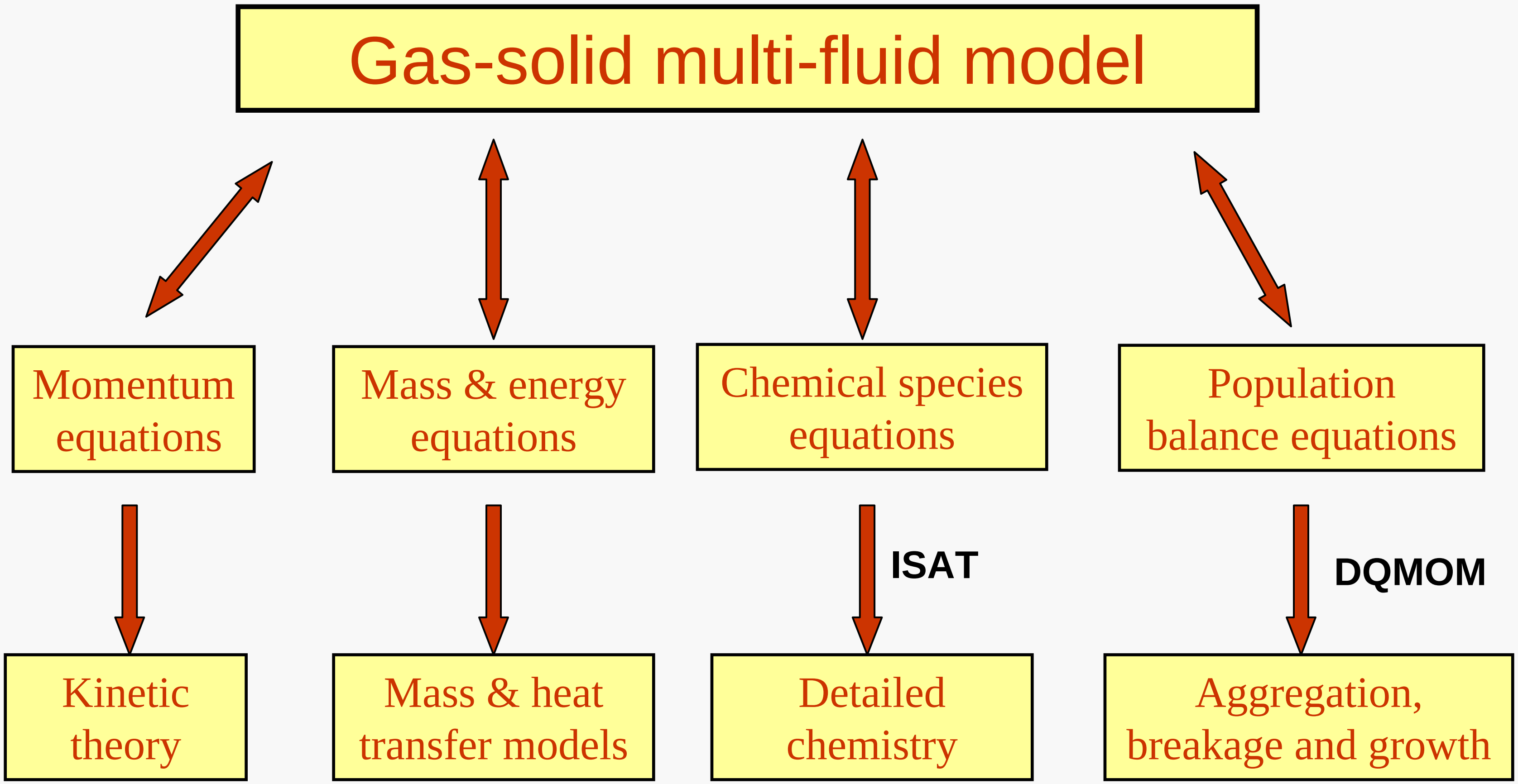
Overview of MFIX



MFIX Governing Equations (I)

- Mass balances

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g) = -\sum_{\alpha=1}^{N} \sum_{n=1}^{N_s} M_{g\alpha n}$$

$$\frac{\partial}{\partial t}(\varepsilon_{s\alpha} \rho_{s\alpha}) + \nabla \cdot (\varepsilon_{s\alpha} \rho_{s\alpha} \mathbf{u}_{s\alpha}) = \sum_{n=1}^{N_s} M_{g\alpha n}$$

Mass transfer from gas to solid phases

- Momentum balances

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \mathbf{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \mathbf{u}_g \mathbf{u}_g) = \nabla \cdot \boldsymbol{\sigma}_g + \sum_{\alpha=1}^{N} \mathbf{f}_{g\alpha} + \varepsilon_g \rho_g \mathbf{g}$$

$$\frac{\partial}{\partial t}(\varepsilon_{s\alpha} \rho_{s\alpha} \mathbf{u}_{s\alpha}) + \nabla \cdot (\varepsilon_{s\alpha} \rho_{s\alpha} \mathbf{u}_{s\alpha} \mathbf{u}_{s\alpha}) = \nabla \cdot \boldsymbol{\sigma}_{s\alpha} - \mathbf{f}_{g\alpha} + \sum_{\beta=1, \beta\neq\alpha}^{N} \mathbf{f}_{\beta\alpha} + \varepsilon_{s\alpha} \rho_{s\alpha} \mathbf{g}$$

Stress tensor | **Interaction with gas and other solid phases** | **Body force**

g: Gas phase
$s\alpha$: Solid phases α=1, N

MFIX Governing Equations (II)

- Thermal energy balances

$$\varepsilon_g \rho_g C_{pg}\left(\frac{\partial T_g}{\partial t} + \mathbf{u}_g \cdot \nabla T_g\right) = -\nabla \cdot \mathbf{q}_g - \sum_{\alpha=1}^{N} H_{g\alpha} - \Delta H_{rg} + H_{wall}(T_{wall} - T_g)$$

$$\varepsilon_{s\alpha} \rho_{s\alpha} C_{ps\alpha}\left(\frac{\partial T_{s\alpha}}{\partial t} + \mathbf{u}_{s\alpha} \cdot \nabla T_{s\alpha}\right) = -\nabla \cdot \mathbf{q}_{s\alpha} + H_{g\alpha} - \Delta H_{rs\alpha}$$

Heat lost to walls

Conductive heat flux | **Heat transfer between phases** | **Heat of reaction**

- Chemical species balances

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g X_{gn}) + \nabla \cdot (\varepsilon_g \rho_g X_{gn} \mathbf{u}_g) = R_{gn} - \sum_{\alpha=1}^{N} M_{g\alpha n}$$

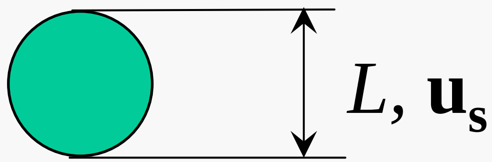
$$\frac{\partial}{\partial t}(\varepsilon_{s\alpha} \rho_{s\alpha} X_{s\alpha n}) + \nabla \cdot (\varepsilon_{s\alpha} \rho_{s\alpha} X_{s\alpha n} \mathbf{u}_{s\alpha}) = R_{s\alpha n} + M_{g\alpha n}$$

Reactions | **Mass transfer**

g: Gas phase
sα: Solid phases α=1, N

Polydisperse Solids Model

- Population balance equation for solid phase



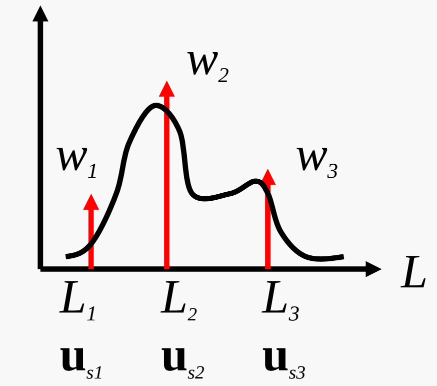
Force acting to accelerate particles

$$\frac{\partial n(L,\mathbf{u}_s;x,t)}{\partial t} + \nabla \cdot \left[\mathbf{u}_s n\left(L,\mathbf{u}_s;\mathbf{x},t\right) \right] + \nabla_{\mathbf{u}_s} \cdot \left[\mathbf{F} n\left(L,\mathbf{u}_s;\mathbf{x},t\right) \right] = S(L,\mathbf{u}_s;x,t)$$

Joint size & velocity distribution function

Aggregation, breakage and chemical reaction

Direct Quadrature Method of Moments



$$\frac{\partial n(L,\mathbf{u}_s;x,t)}{\partial t}+\nabla\cdot\left[\mathbf{u}_s n\left(L,\mathbf{u}_s;\mathbf{x},t\right)\right]+\nabla_{\mathbf{u}_s}\cdot\left[\mathbf{F}n\left(L,\mathbf{u}_s;\mathbf{x},t\right)\right]=S(L,\mathbf{u}_s;x,t)$$

Integrate out solid velocity

$$\frac{\partial n(L;x,t)}{\partial t}+\nabla\cdot\left[\langle\mathbf{u}_s\,|\,L\rangle\; n\left(L;\mathbf{x},t\right)\right]=S(L;x,t)$$

Use distribution function

$$n\left(L;\mathbf{x},t\right)=\sum_{\alpha=1}^{N}\omega_\alpha\left(\mathbf{x},t\right)\delta\left[L-L_\alpha\left(\mathbf{x},t\right)\right]$$

$$\frac{\partial}{\partial t}\left[\sum_{\alpha=1}^{N}\omega_\alpha\delta(L-L_\alpha)\right]+\nabla\cdot\left[\mathbf{u}_{s\alpha}\sum_{\alpha=1}^{N}\omega_\alpha\delta(L-L_\alpha)\right]=S(L;x,t)$$

Simplify equation

$$\begin{cases}\nabla\cdot\left(\mathbf{u}_\alpha\omega_\alpha\right)=a_\alpha\\ \dfrac{\partial\omega_\alpha L_\alpha}{\partial t}+\nabla\cdot\left(\mathbf{u}_\alpha\omega_\alpha L_\alpha\right)=b_\alpha\end{cases}$$

$$\sum_{\alpha=1}^{N}\left[\delta(L-L_\alpha)a_\alpha-\delta'(L-L_\alpha)(b_\alpha-L_\alpha a_\alpha)\right]=S(L;x,t)$$

Moment transform

$$m_k\left(\mathbf{x},t\right)=\int_0^{+\infty}n\left(L;\mathbf{x},t\right)L^k dL\approx\sum_{\alpha=1}^{N}\omega_\alpha L_\alpha^k$$

$$\sum_{\alpha=1}^{N}\left[a_\alpha L_\alpha^k+kL_\alpha^{k-1}(b_\alpha-L_\alpha a_\alpha)\right]=\overline{S}_k(x,t)$$

$$\mathbf{Ax}=\mathbf{b}$$

Modifications to MFIX

- Relation between volume fractions and weights:

$$\varepsilon_{s\alpha} = k_v L_\alpha^3 \omega_\alpha$$

$\boldsymbol{k_v}$**: volumetric shape factor**

- Transport equations for volume fractions and lengths:

$$\frac{\partial(\varepsilon_{s\alpha}\rho_{s\alpha})}{\partial t} + \nabla\cdot(\varepsilon_{s\alpha}\rho_{s\alpha}\mathbf{u}_{s\alpha}) = 3k_v\rho_{s\alpha}L_\alpha^2 b_\alpha - 2k_v\rho_{s\alpha}L_\alpha^3 a_\alpha$$

$$\frac{\partial(\varepsilon_{s\alpha}L_\alpha\rho_{s\alpha})}{\partial t} + \nabla\cdot(\varepsilon_{s\alpha}L_\alpha\rho_{s\alpha}\mathbf{u}_{s\alpha}) = 4k_v\rho_{s\alpha}L_\alpha^3 b_\alpha - 3k_v\rho_{s\alpha}L_\alpha^4 a_\alpha$$

DQMOM Source Terms

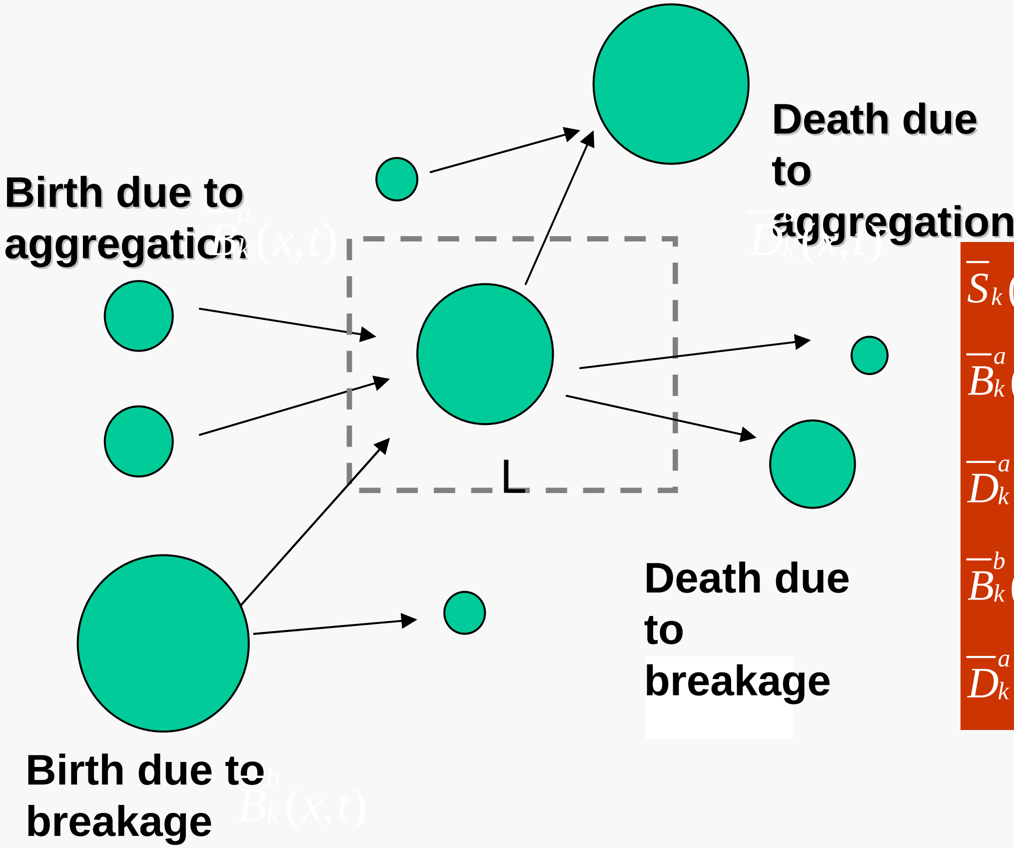
$$\mathbf{Ax} = \mathbf{b}$$

$$\mathbf{A} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ -L_1^2 & -L_2^2 & 2L_1 & 2L_2 \\ -2L_1^3 & -2L_2^3 & 3L_1^2 & 3L_2^2 \end{pmatrix} \qquad \mathbf{x} = \begin{pmatrix} a_1 \\ a_2 \\ b_1 \\ b_2 \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} \overline{S}_0 \\ \overline{S}_1 \\ \overline{S}_2 \\ \overline{S}_3 \end{pmatrix}$$

Matrix **A** relates moments to weights and lengths

Source term **x** is obtained by forcing moments to be exact

Aggregation and Breakage



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

$$\overline{B}_k^{a}(x,t) = \frac{1}{2}\int_0^{+\infty} n(\lambda;x,t)\int_0^{+\infty}\beta(u,\lambda)(u^3+\lambda^3)^{k/3} n(u;x,t)\,du\,d\lambda$$

$$\overline{D}_k^{a}(x,t) = \int_0^{+\infty} L^k n(L;x,t)\int_0^{+\infty}\beta(L,\lambda) n(\lambda;x,t)\,d\lambda\,dL$$

$$\overline{B}_k^{b}(x,t) = \int_0^{+\infty} L^k \int_0^{+\infty} a(\lambda) b(L\,|\,\lambda) n(\lambda;x,t)\,d\lambda\,dL$$

$$\overline{D}_k^{a}(x,t) = \int_0^{+\infty} L^k a(L) n(L;x,t)\,dL$$

Apply DQMOM

$$\overline{S}_k(x,t) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\omega_i\omega_j (L_i^{\,3}+L_j^{\,3})^{k/3}\beta_{ij} - \sum_{i=1}^{N}\sum_{j=1}^{N}\omega_i\omega_j L_i^{\,k}\beta_{ij} + \sum_{i=1}^{N}\omega_i a_i \overline{b}_i^{(k)} - \sum_{i=1}^{N}\omega_i L_i^{\,k} a_i$$

Aggregation and Breakage Kernels

- Aggregation and breakage kernels are obtained from kinetic theory

Number of collisions:

$$N_{ij} = \pi\omega_i\omega_j\sigma_{ij}^3 g_{ij}\left[\frac{4}{\sigma_{ij}}\left(\frac{\theta_s}{\pi}\frac{m_i+m_j}{2m_i m_j}\right)^{\frac{1}{2}} - \frac{2}{3}(\nabla\cdot\mathbf{u}_s)\right]$$

Aggregation kernel:

$$\beta_{ij} = \frac{N_{ij}}{\omega_i\omega_j}\psi_a$$

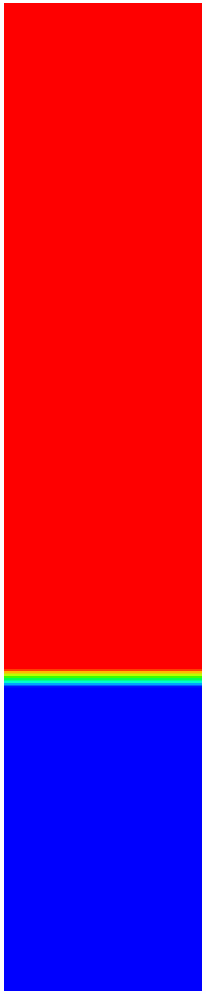
Breakage kernel:

$$a_i = \sum_i \frac{N_{ij}}{\omega_i}\psi_b$$

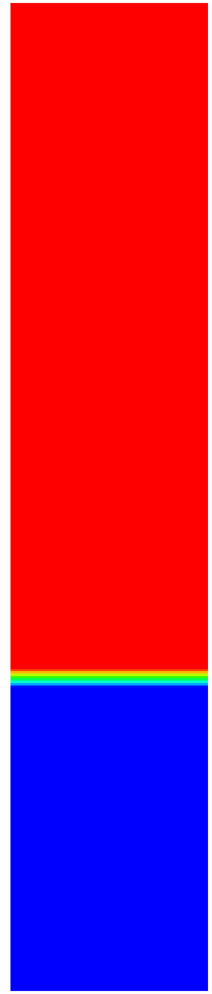
Efficiencies (ψ_a and ψ_b) depend on temperature, particle size, etc.

PSD Effect on Fluidization

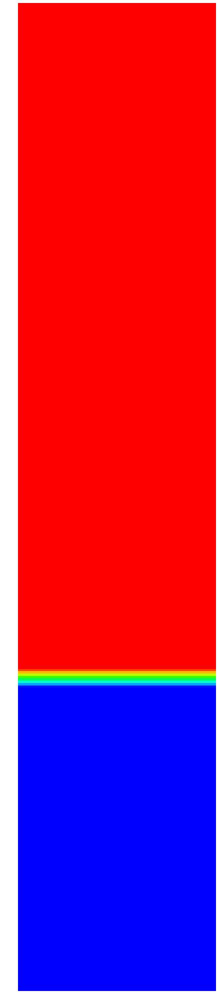
No aggregation and breakage



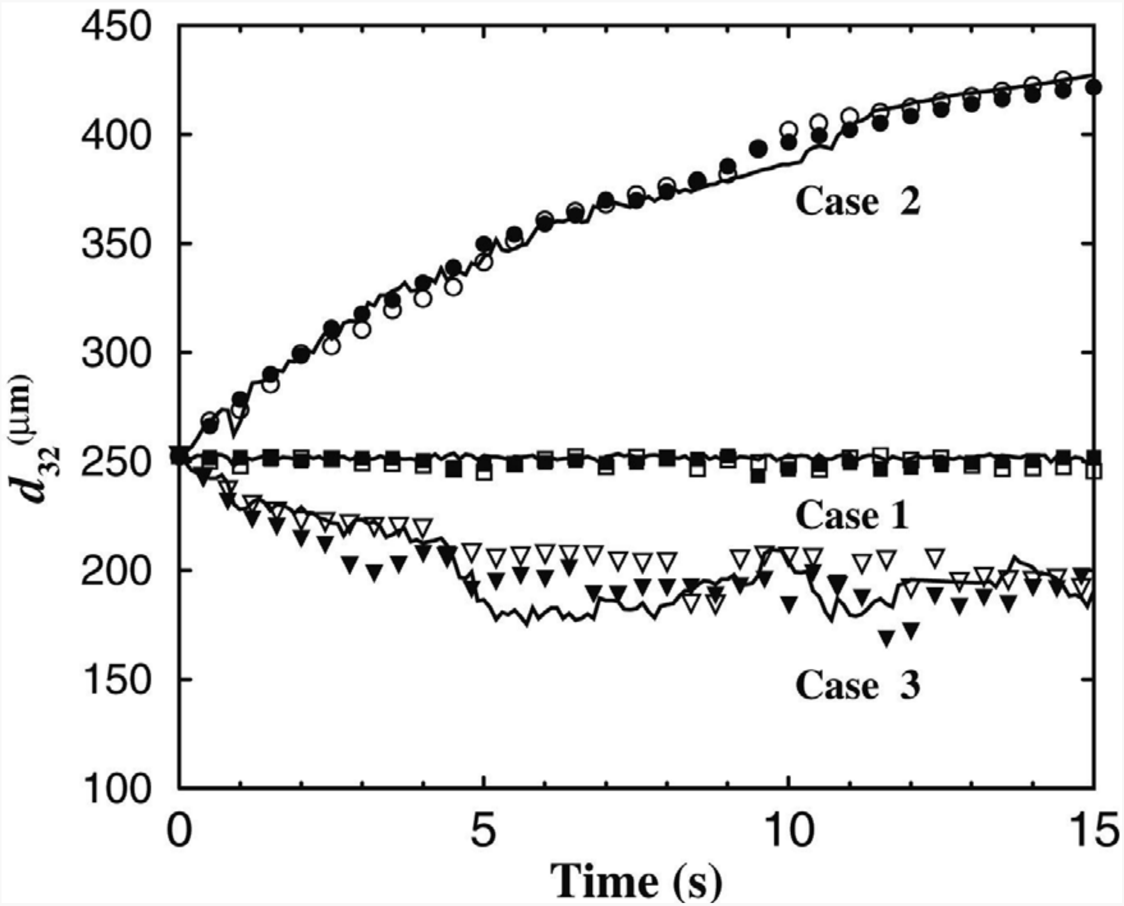
Breakage dominant
average size decreases, FB expands



Aggregation dominant
average size Increases, FB defluidizes



Volume-Average Mean Diameter



N = 2 filled symbols
N = 3 empty symbols
N = 4 lines

Case 1

$\beta = 0;\ a = 0$

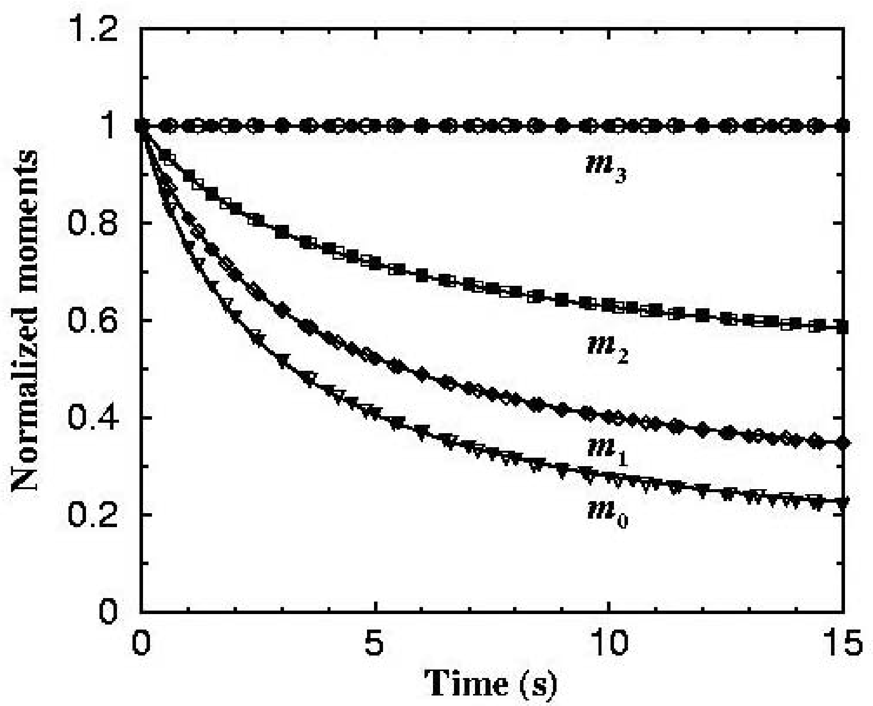
Case 2

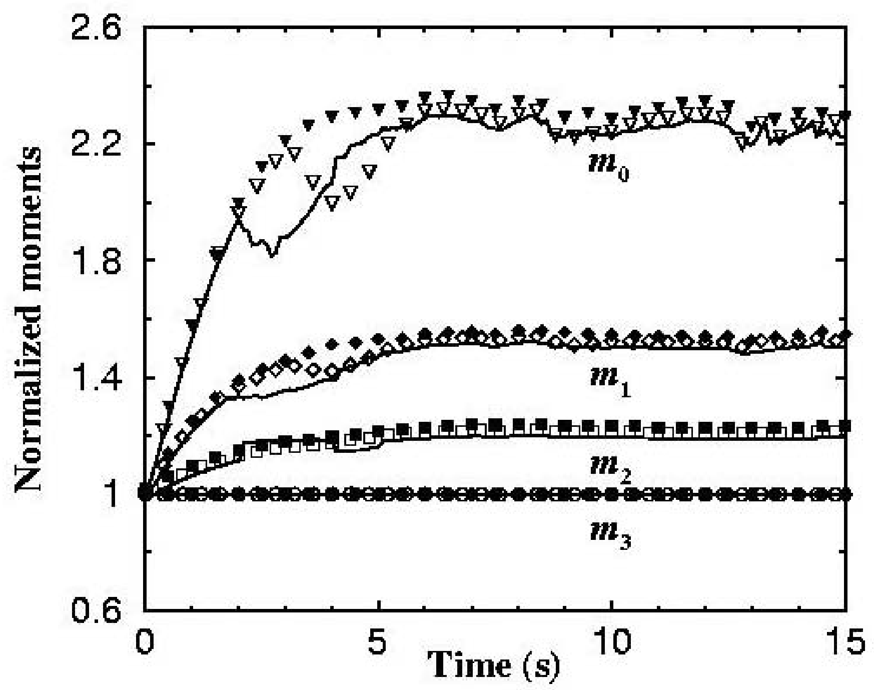
$\beta = 1\times10^{-5}\, m^3/s;$
$a = 0.1\ s^{-1}$

Case 3

$\beta = 1\times10^{-5}\, m^3/s;$
$a = 1\ s^{-1}$

Volume-Average Normalized Moments





N = 2 filled symbols
N = 3 empty symbols
N = 4 lines

$$m_k(\mathbf{x},t) = \int_0^{+\infty} n(L;\mathbf{x},t)L^k dL \approx \sum_{\alpha=1}^{N} \omega_\alpha L_\alpha^k$$

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Extension to Energy/Species Balances

- Thermal energy balance

$$\varepsilon_{s\alpha}\rho_{s\alpha}C_{ps\alpha}\left(\frac{\partial T_{s\alpha}}{\partial t}+\mathbf{u}_{s\alpha}\cdot\nabla T_{s\alpha}\right)=-\nabla\cdot\mathbf{q}_{s\alpha}+H_{g\alpha}-\Delta H_{rs\alpha}$$
$$+k_v\rho_s L_\alpha^3 C_{ps} c_{T,\alpha}-k_v\rho_s L_\alpha^3 C_{ps} T_{s\alpha} a_\alpha$$

Changes due to aggregation and breakage

Multi-variate DQMOM

$$\Delta H_{rs\alpha}=\varepsilon_{s\alpha}R_{s\alpha,C_2}\Delta H_r$$

$$R_{s\alpha,C_2}=-k_p[c^*]P_{C_2}^{\prime\prime\prime}$$

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   – Coupling with CFD
2. Population Balances in CFD
   – Population Balance Equation
   – Direct Solvers
   – Quadrature Methods
3. Implementation for Gas-Solid Flow
   – Overview of MFIX
   – Polydisperse Solids Model
   – Application of DQMOM
4. **Two Open Problems**

Two Open Problems

1. How to extend DQMOM to systems with unknown fluxes at boundaries in phase space?

Model problem: pure evaporation

$$\frac{\partial n}{\partial t} = \frac{\partial n}{\partial v} \quad \Longrightarrow \quad \frac{dm_k}{dt} = -\delta_{k,0}\, n(0,t) - k m_{k-1}$$

How can we estimate it?

Estimate flux in DQMOM variables, test with exact solutions:

Define vectors:

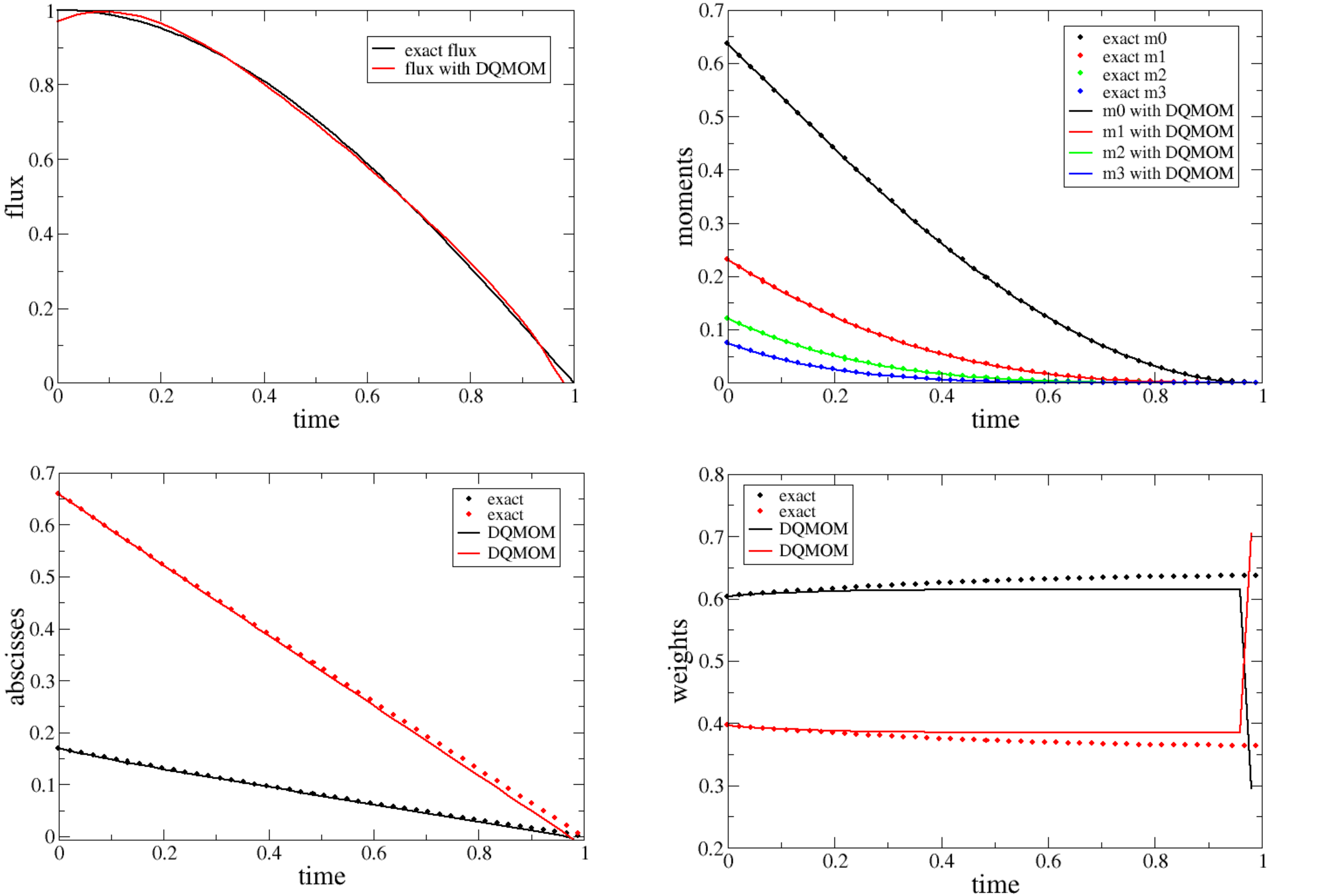
$$x_\alpha = w_\alpha v_\alpha / m_0$$

$$\dot{\mathbf{x}} = d\mathbf{x}/dt$$

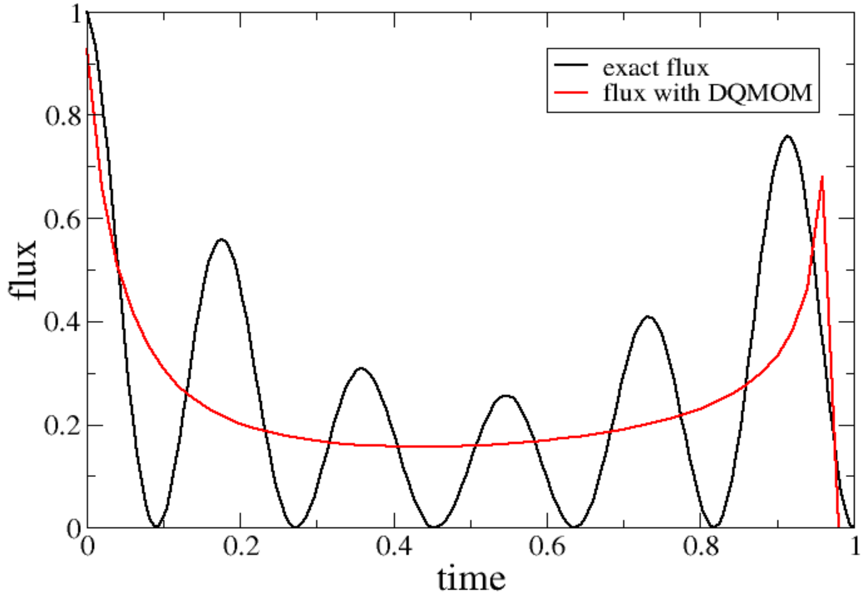
Define "cross product": $\mathbf{c} = \dot{\mathbf{x}} \times \mathbf{x}$

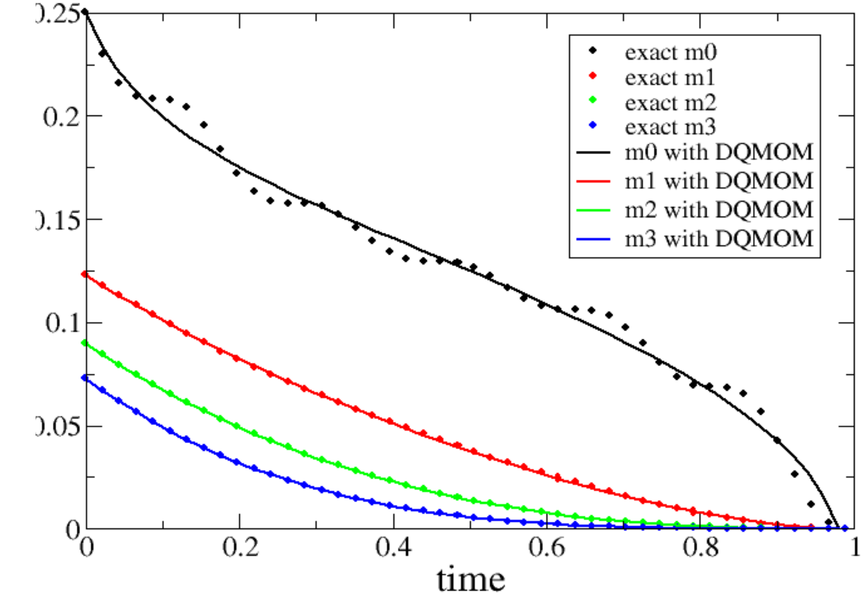
Linear constraint: $\sum c_\alpha = 0$

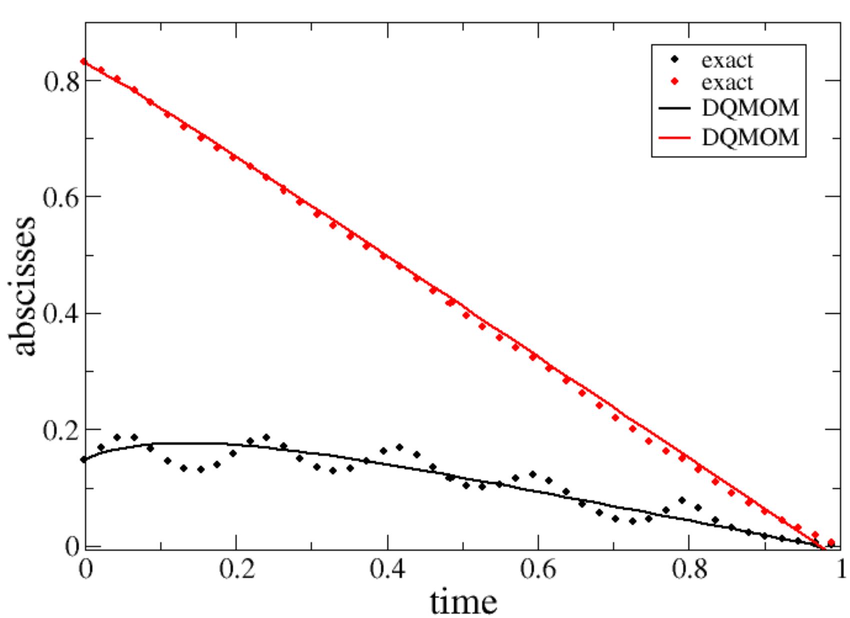
Simple case with monotone flux ($N = 2$):

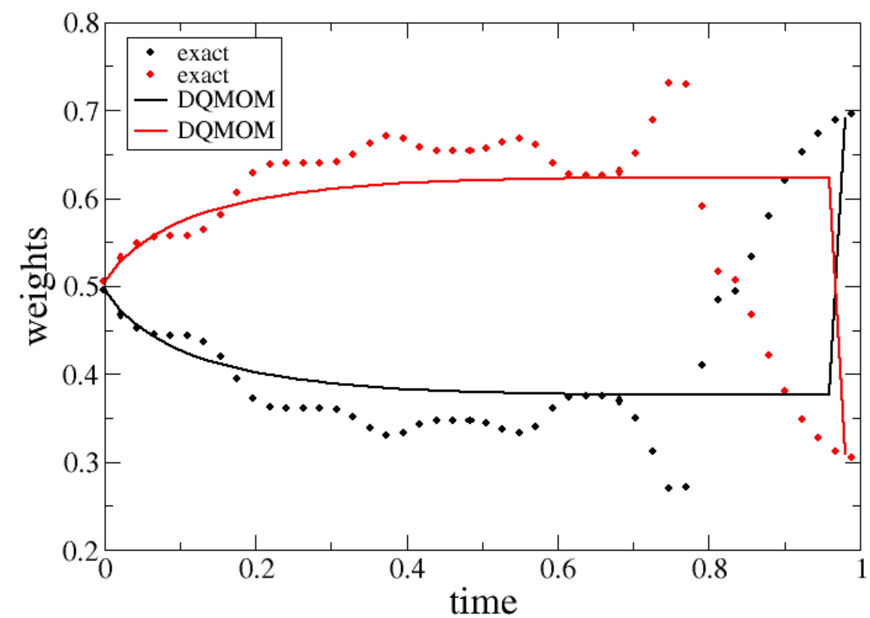


Harder case with multimode flux (N = 2):

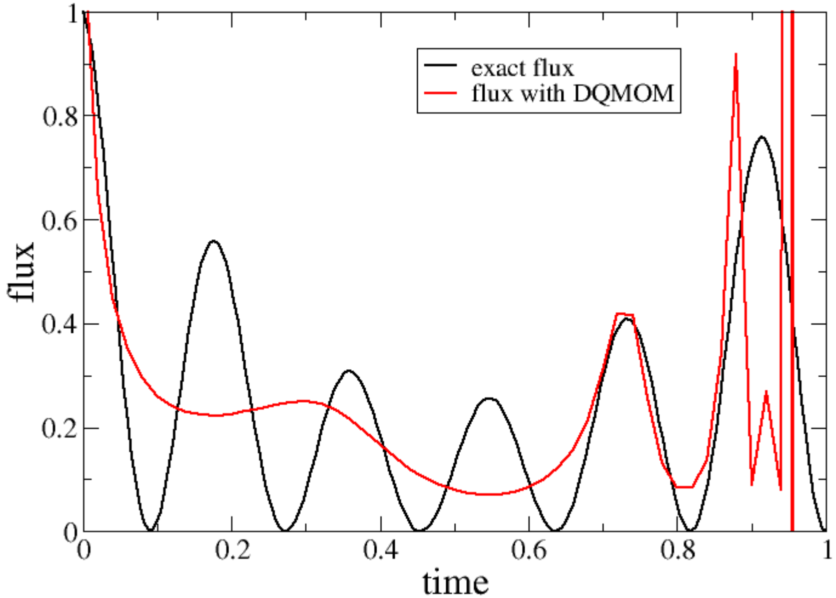


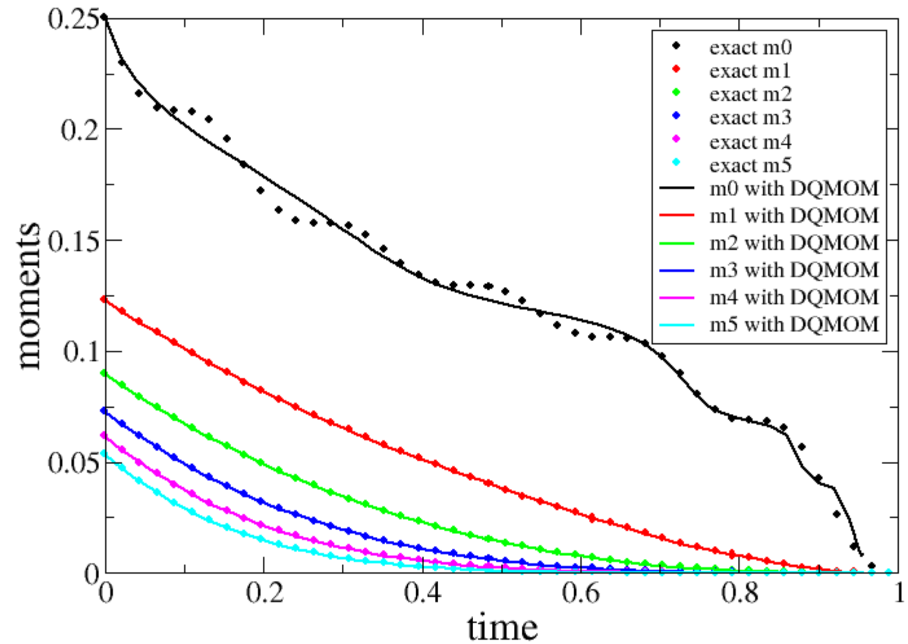


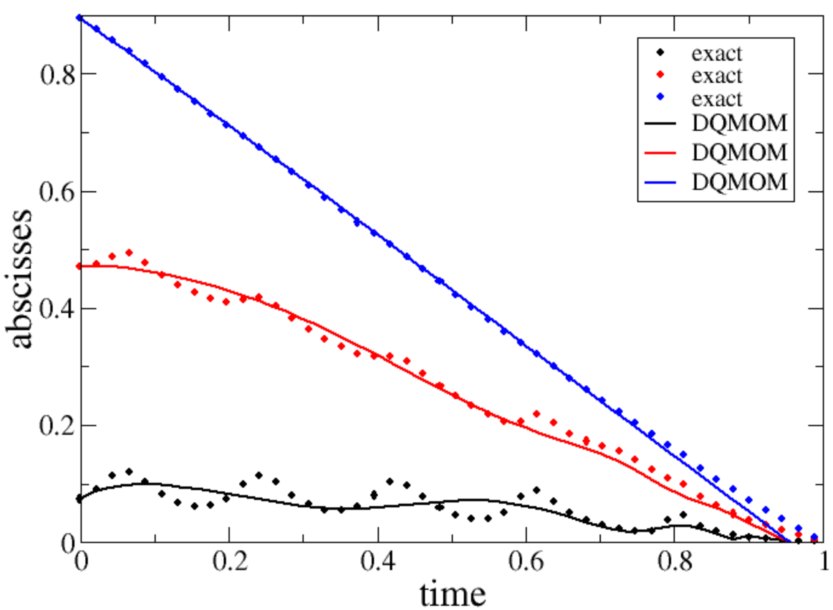


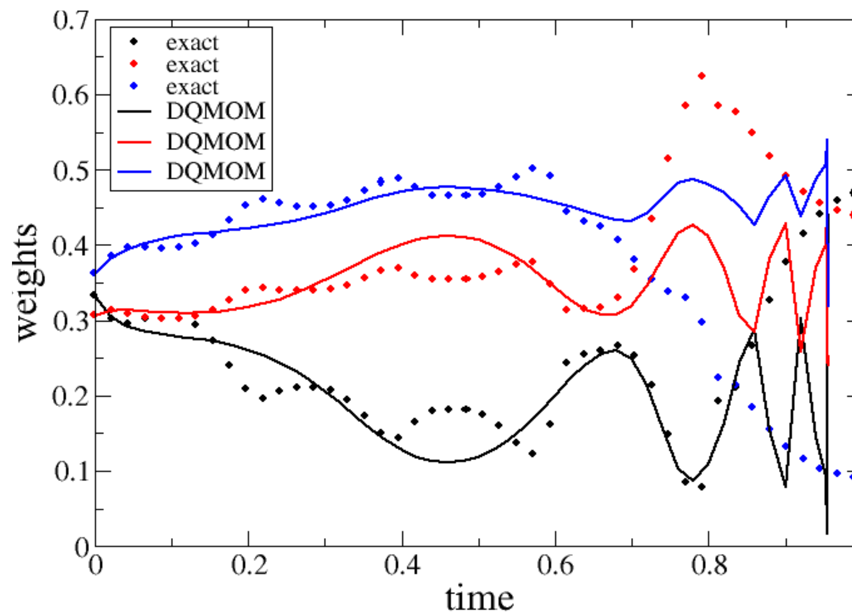


Harder case with N = 3:









Two Open Problems

2. What is “best” choice of moments for multivariate DQMOM?

Model problem: homogeneous aggregation

$$\frac{dw_n}{dt} = a_n$$

$$\frac{dw_n v_n}{dt} = b_n$$

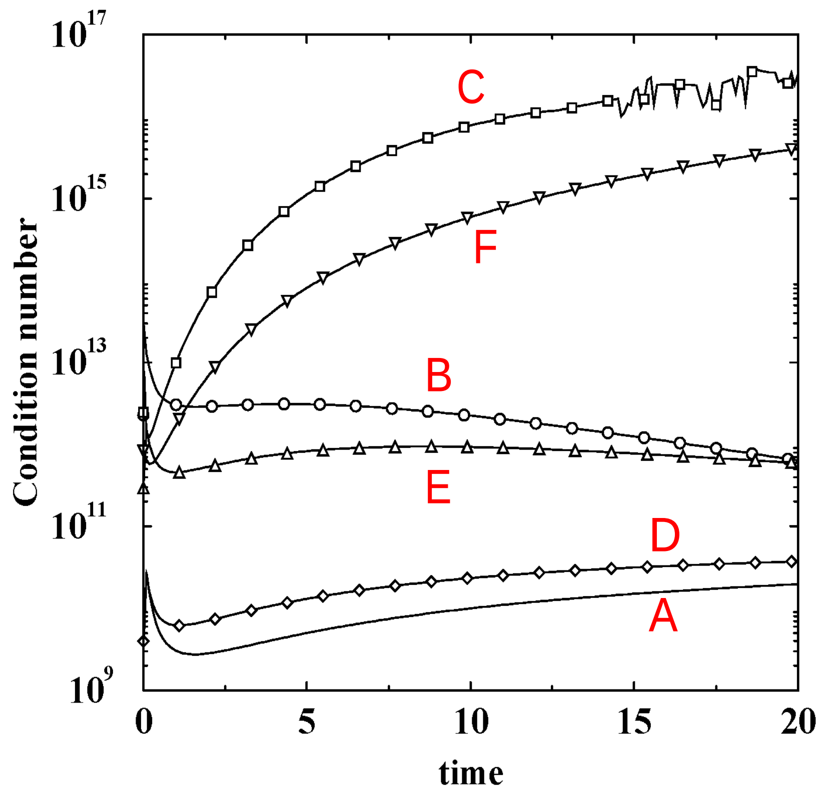
$$\frac{dw_n a_n}{dt} = c_n$$

Aggregation

Aggregation + sintering

$\langle v^k a^l \rangle$ Moments (mass ***k***=1, ***l***=0; area ***k***=0, ***l***=1)

- Choice of moments affects the condition of matrix



	Set A4		Set B4		Set C4		Set D4		Set E4		Set F4	
	k	*l*	*k*	*l*	*k*	*l*	*k*	*l*	*k*	*l*	*k*	*l*
1	0	0	0	0	0	0	0	0	0	0	0	0
2	1/3	0	1/3	0	1/3	1/3	1/3	0	0	1/3	1/4	0
3	2/3	0	2/3	0	2/3	2/3	2/3	0	0	2/3	1/3	0
4	1	0	1	0	1	1	1	0	0	1	1/2	0
5	4/3	0	4/3	0	4/3	4/3	4/3	0	0	4/3	1	0
6	5/3	0	5/3	0	5/3	5/3	5/3	0	0	5/3	2	0
7	2	0	2	0	2	2	2	0	0	2	3	0
8	7/3	0	7/3	0	7/3	7/3	7/3	0	0	7/3	4	0
9	0	1/3	0	1/3	2/3	1/3	0	1/3	1/3	0	0	1/4
10	0	2/3	0	1	1	2/3	2/3	1/3	2/3	0	0	1/3
11	0	1	0	5/3	4/3	1	4/3	1/3	1	0	0	1/2
12	0	4/3	0	7/3	5/3	4/3	2	1/3	4/3	0	0	1

All choices yield nearly same weights and abscissas
Choose moments with lowest condition number?

Another example: Williams' Spray Equation

$$\partial_t f + \mathbf{u} \cdot \partial_{\mathbf{x}} f + \partial_v (R_v f) + \partial_{\mathbf{u}} \cdot (\mathbf{F} f) = \Gamma$$

$f(v, \mathbf{u}; \mathbf{x}, t) =$ volume, velocity number density function

$R_v =$ evaporation rate

$\mathbf{F} =$ drag force

$\Gamma = Q^- + Q^+ =$ coalesence operator

$$Q^- = -\int\int B(|\mathbf{u}-\mathbf{u}^*|, v, v^*) f(v, \mathbf{u}) f(v^*, \mathbf{u}^*)\, dv^*\, d\mathbf{u}^*$$

$$Q^+ = \frac{1}{2}\int\int B(|\mathbf{u}^\diamond-\mathbf{u}^*|, v^\diamond, v^*) f(v^\diamond, \mathbf{u}^\diamond) f(v^*, \mathbf{u}^*) J\, dv^*\, d\mathbf{u}^*$$

Coefficients depend on choice of 5*N* moments:

$$\langle v^k u_1^l u_2^m u_3^p \rangle$$

Condition number of **A** depends on choice of ***k, l, m, p***

In general, **A** matrix will become singular if $1 < l + m + p$

Choose ***l, m, p*** **= (0,1)** and vary ***k*** to yield **5*N*** distinct moments

Number: $(k, l, m, p) = 0$

Mass: $k = 1, (l, m, p) = 0$

X-Mom: $k = 1, l = 1$ Y-Mom: $k = 1, m = 1$ Z-Mom: $k = 1, p = 1$

Is there a general method for choosing moments?