Experimental validation of CFD models for polydisperse fluidized powders based on the quadrature methods of moments

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Outline

- The Generalized Population Balance approach
- QMOM and DQMOM
  - Mono-dispersed case
  - Binary case
- Experimental and simulation set-up for mixing and segregation
- Results
- Conclusions

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Introduction

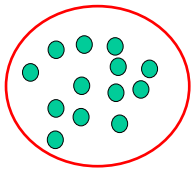
- Quadrature methods have been proposed in 1997 by Robert McGraw
- QMOM has been validated and applied to the simulation of many particulate systems coupled with Eulerian-Eulerian volume-averaged approaches
- DQMOM has been proposed in 2003; it was shown to be equivalent to QMOM for low Stokes numbers

Topics of this work:

- QMOM/DQMOM identify a new class of methods that do not need volume average
- QMOM and DQMOM are identical also for high Stokes number flows
- Application to mixing and segregation in fluidized beds: comparison with experimental data

Generalized Population Balance Equation

- A particulate multiphase system can be characterized in terms of a NUMBER DENSITY FUNCTION:



Particle velocity

$$n(L, \mathbf{U}_\mathrm{p}, \mathbf{U}_\mathrm{c}; \mathbf{x}, t)\, \mathrm{d}L\, \mathrm{d}\mathbf{U}_\mathrm{p}\, \mathrm{d}\mathbf{U}_\mathrm{c}\, \mathrm{d}\mathbf{x}$$

Particle size

Fluid velocity "seen" by the particle

- … or by a VOLUME DENSITY FUNCTION:

$$\phi(L, \mathbf{U}_\mathrm{p}, \mathbf{U}_\mathrm{c}; \mathbf{x}, t) = k_v L^3 n(L, \mathbf{U}_\mathrm{p}, \mathbf{U}_\mathrm{c}; \mathbf{x}, t)$$

Particle shape factor

Generalized Population Balance Equation

- Governed by a Generalized Population Balance Equation

Particle convection

Particle continuous growth

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x_i}(U_{\mathrm{p}i}\phi) + \frac{\partial}{\partial L}(G\phi) - \frac{3G}{L}\phi + \frac{\partial}{\partial U_{\mathrm{p}i}}(A_{\mathrm{p}i}\phi) + \frac{\partial}{\partial U_{\mathrm{c}i}}(A_{\mathrm{c}i}\phi) = h(L, \mathbf{U}_\mathrm{p}, \mathbf{U}_\mathrm{c}; \mathbf{x}, t)$$

Particle acceleration

Fluid acceleration (seen by the particle)

Particle collision + nucleation

$$\frac{\partial \phi}{\partial t} + \nabla_\mathbf{x}(\mathbf{U}_\mathrm{p}\phi) + \nabla_L(G\phi) - \frac{3G}{L}\phi + \nabla_{\mathbf{U}_\mathrm{p}}(\mathbf{A}_\mathrm{p}\phi) + \nabla_{\mathbf{U}_\mathrm{c}}(\mathbf{A}_\mathrm{c}\phi) = h(L, \mathbf{U}_\mathrm{p}, \mathbf{U}_\mathrm{c}; \mathbf{x}, t)$$

Vectorial notation

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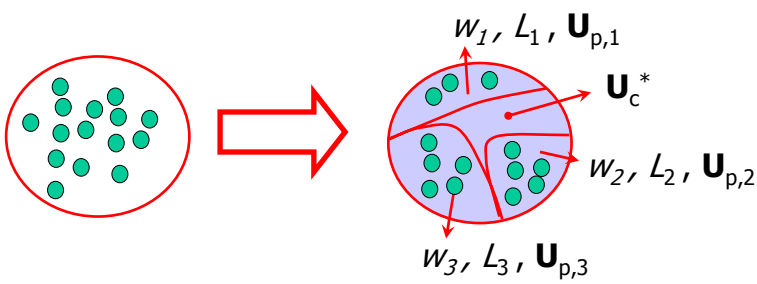
Quadrature approximation

- The NDF can be described as a summation of Dirac delta functions

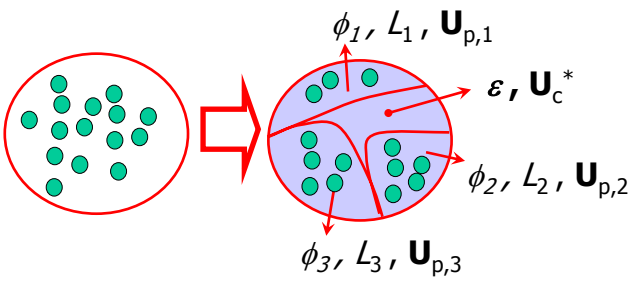
$$n(L, \mathbf{U}_\mathrm{p}, \mathbf{U}_\mathrm{c}; \mathbf{x}, t) = \sum_{\alpha=1}^{N} w_\alpha \delta(L - L_\alpha)\delta(\mathbf{U}_\mathrm{p} - \mathbf{U}_{\mathrm{p},\alpha})\delta(\mathbf{U}_\mathrm{c} - \mathbf{U}_\mathrm{c}^*)$$



Quadrature approximation

- The VDF can be described as a summation of Dirac delta functions

$$\phi(L, \mathbf{U}_\mathrm{p}, \mathbf{U}_\mathrm{c}; \mathbf{x}, t) = \sum_{\alpha=1}^{N} \phi_\alpha \delta(L - L_\alpha) \prod_{i=1}^{3} \delta(U_{\mathrm{p}i} - U_{\mathrm{p}i,\alpha}) \prod_{i=1}^{3} \delta(U_{\mathrm{c}i} - U^*_{\mathrm{c}i})$$



$$\phi_\alpha = w_\alpha k_v L_\alpha^3$$

$$\phi_t(\mathbf{x}, t) = \sum_{\alpha=1}^{N} \phi_\alpha$$

$$\varepsilon(\mathbf{x}, t) = 1 - \phi_t(\mathbf{x}, t)$$

Quadrature approximation

- The GPBE is therefore solved in terms of the evolution of each node of the quadrature approximation $(\text{for } \alpha \in 0, ..., N)$

$$\begin{aligned}
\frac{\partial}{\partial t}(\phi_\alpha) + \frac{\partial}{\partial x_i}(\phi_\alpha U_{\mathrm{p}i,\alpha}) &\equiv a_\alpha \\
\frac{\partial}{\partial t}(\phi_\alpha L_\alpha) + \frac{\partial}{\partial x_i}(\phi_\alpha U_{\mathrm{p}i,\alpha} L_\alpha) &\equiv b_\alpha \\
\frac{\partial}{\partial t}(\phi_\alpha U_{\mathrm{p}j,\alpha}) + \frac{\partial}{\partial x_i}(\phi_\alpha U_{\mathrm{p}i,\alpha} U_{\mathrm{p}j,\alpha}) &\equiv c_{j,\alpha} \quad j \in 1, 2, 3 \\
\frac{\partial}{\partial t}(\phi_\alpha U^*_{\mathrm{c}j}) + \frac{\partial}{\partial x_i}(\phi_\alpha U_{\mathrm{p}i,\alpha} U^*_{\mathrm{c}j}) &\equiv d_{j,\alpha} \quad j \in 1, 2, 3
\end{aligned}$$

Quadrature approximation

- The source terms are calculated by forcing some moments of the VDF to be correctly predicted:

$$m_{l,\mathbf{k},\mathbf{h}}(\mathbf{x},t) = \int_{\Omega_L}\int_{\Omega_{\mathbf{U}_\mathrm{p}}}\int_{\Omega_{\mathbf{U}_\mathrm{c}}} \phi(L,\mathbf{U}_\mathrm{p},\mathbf{U}_\mathrm{c};\mathbf{x},t) L^l \mathbf{U}_\mathrm{p}^{\mathbf{k}} \mathbf{U}_\mathrm{c}^{\mathbf{h}} \,\mathrm{d}L\,\mathrm{d}\mathbf{U}_\mathrm{p}\,\mathrm{d}\mathbf{U}_\mathrm{c}$$

Order of the moment with respect to **particle size *L***

$$m_{l,\mathbf{k},\mathbf{h}}$$

$\mathbf{h} = (h_1, h_2, h_3)$
Order of the moment with respect to **fluid velocity $\mathbf{U}_\mathbf{c}$**

$\mathbf{k} = (k_1, k_2, k_3)$
Order of the moment with respect to **particle velocity $\mathbf{U}_\mathrm{p}$**

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Mono-dispersed system ($N = 1$)

- If only one node is used:

$$\boxed{\begin{array}{l} l=0, k_1=0, k_2=0, k_3=0, h_1=0, h_2=0, h_3=0, \\ l=1, k_1=0, k_2=0, k_3=0, h_1=0, h_2=0, h_3=0, \end{array}}$$

$$\frac{\partial}{\partial t}(\phi_1) + \nabla(\mathbf{U}_{\mathrm{p},1}\phi_1) = a_1,$$

particle growth rate

$$\frac{\partial}{\partial t}(\phi_1 L_1) + \nabla(\phi_1 \mathbf{U}_{\mathrm{p},1} L_1) = b_1^* + \phi_1 G(L_1, \mathbf{U}_{\mathrm{p},1}, \mathbf{U}_{\mathrm{c}}),$$

$$\frac{\partial}{\partial t}(\phi_1 \mathbf{U}_{\mathrm{p},1}) + \nabla(\phi_1 \mathbf{U}_{\mathrm{p},1}\mathbf{U}_{\mathrm{p},1}) = \mathbf{c}_1^* + \phi_1 \mathbf{A}_{\mathrm{p}}(L_1, \mathbf{U}_{\mathrm{p},1}, \mathbf{U}_{\mathrm{c}}),$$

particle continuous acceleration

$$\boxed{\begin{array}{l} l=0, k_1=1, k_2=0, k_3=0, h_1=0, h_2=0, h_3=0, \\ l=0, k_1=0, k_2=1, k_3=0, h_1=0, h_2=0, h_3=0, \\ l=0, k_1=0, k_2=0, k_3=1, h_1=0, h_2=0, h_3=0, \end{array}}$$

Mono-dispersed system ($N = 1$)

- Final equations (identical to volume-averaged equations!):

nucleation

$$\frac{\partial}{\partial t}(\varrho_{\mathrm{p}}\phi_1) + \nabla(\varrho_{\mathrm{p}}\phi_1 \mathbf{U}_{\mathrm{p},1}) = \varrho_{\mathrm{p}} S_{0,0,0} + \frac{3\varrho_{\mathrm{p}}\phi_1}{L_1} G(L_1, \mathbf{U}_{\mathrm{p},1}, \mathbf{U}_{\mathrm{c}}),$$

nucleation and collisions **particle growth**

$$\frac{\partial}{\partial t}(\varrho_{\mathrm{p}}\phi_1 L_1) + \nabla(\varrho_{\mathrm{p}}\phi_1 \mathbf{U}_{\mathrm{p},1} L_1) = \varrho_{\mathrm{p}} S_{1,0,0} + 4\varrho_{\mathrm{p}}\phi_1 G(L_1, \mathbf{U}_{\mathrm{p},1}, \mathbf{U}_{\mathrm{c}}),$$

nucleation and collisions

$$\frac{\partial}{\partial t}(\varrho_{\mathrm{p}}\phi_1 \mathbf{U}_{\mathrm{p},1}) + \nabla(\varrho_{\mathrm{p}}\phi_1 \mathbf{U}_{\mathrm{p},1}\mathbf{U}_{\mathrm{p},1}) = \varrho_{\mathrm{p}} \mathbf{S}_{0,1,0} + \frac{3\varrho_{\mathrm{p}}\phi_1}{L_1} G(L_1, \mathbf{U}_{\mathrm{p},1}, \mathbf{U}_{\mathrm{c}})\mathbf{U}_{\mathrm{p},1}$$
$$- \phi_1 \nabla p + \phi_1 \varrho_{\mathrm{p}} \mathbf{g} + \phi_1 \varepsilon \frac{3}{4} C_D \varrho_{\mathrm{c}} \frac{||\mathbf{U}_{\mathrm{c}} - \mathbf{U}_{\mathrm{p},1}||(\mathbf{U}_{\mathrm{c}} - \mathbf{U}_{\mathrm{p},1})}{L_1}.$$

particle acceleration due to buoyancy, gravity and drag forces

Mono-dispersed system ($N = 1$)

REMINDER!!!

What is S ???

$$S_{l,\mathbf{k},\mathbf{h}}(\mathbf{x},t) = \int_{\Omega_L}\int_{\Omega_{\mathbf{U}_\mathrm{p}}}\int_{\Omega_{\mathbf{U}_\mathrm{c}}} h(L,\mathbf{U}_\mathrm{p},\mathbf{U}_\mathrm{c};\mathbf{x},t)L^l\mathbf{U}_\mathrm{p}^{\mathbf{k}}\mathbf{U}_\mathrm{c}^{\mathbf{h}}\,\mathrm{d}L\,\mathrm{d}\mathbf{U}_\mathrm{p}\,\mathrm{d}\mathbf{U}_\mathrm{c},$$

Particle collision
+ nucleation

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DQMOM - Binary system ($N = 2$)

- The first four moments (with respect to particle size) are conserved:

$$m_{0,\mathbf{0},\mathbf{0}},\ m_{1,\mathbf{0},\mathbf{0}},\ m_{2,\mathbf{0},\mathbf{0}} \text{ and } m_{3,\mathbf{0},\mathbf{0}}$$

$$\frac{\partial}{\partial t}(\phi_1) + \nabla(\mathbf{U}_{\mathrm{p},1}\phi_1) = a_1,$$

$$\frac{\partial}{\partial t}(\phi_2) + \nabla(\mathbf{U}_{\mathrm{p},2}\phi_2) = a_2,$$

$$\frac{\partial}{\partial t}(\phi_1 L_1) + \nabla(\phi_1 \mathbf{U}_{\mathrm{p},1} L_1) = b_1^* + \phi_1 G(L_1, \mathbf{U}_{\mathrm{p},1}, \mathbf{U}_{\mathrm{c}}),$$

$$\frac{\partial}{\partial t}(\phi_2 L_2) + \nabla(\phi_1 \mathbf{U}_{\mathrm{p},2} L_2) = b_2^* + \phi_2 G(L_2, \mathbf{U}_{\mathrm{p},2}, \mathbf{U}_{\mathrm{c}}),$$

$$\boxed{\begin{array}{l} l = 0, k_1 = 0, k_2 = 0, k_3 = 0 \\ l = 1, k_1 = 0, k_2 = 0, k_3 = 0 \\ l = 2, k_1 = 0, k_2 = 0, k_3 = 0 \\ l = 3, k_1 = 0, k_2 = 0, k_3 = 0 \end{array}}$$

DQMOM - Binary system ($N = 2$)

- It can be solved analytically:

$$\begin{aligned}
a_1 &= \frac{S_{0,\mathbf{0},\mathbf{0}}(3L_1 - L_2)L_2^2}{(L_1 - L_2)^3} - \frac{6S_{1,\mathbf{0},\mathbf{0}}L_1L_2}{(L_1 - L_2)^3} + \frac{3S_{2,\mathbf{0},\mathbf{0}}(L_1 + L_2)}{(L_1 - L_2)^3} - \frac{2S_{3,\mathbf{0},\mathbf{0}}}{(L_1 - L_2)^3} + \frac{3\phi_1 G(L_1, \mathbf{U}_{\mathrm{p},1}, \mathbf{U}_{\mathrm{c}})}{L_1} \\
a_2 &= \frac{S_{0,\mathbf{0},\mathbf{0}}(L_1 - 3L_2)L_1^2}{(L_1 - L_2)^3} + \frac{6S_{1,\mathbf{0},\mathbf{0}}L_1L_2}{(L_1 - L_2)^3} - \frac{3S_{2,\mathbf{0},\mathbf{0}}(L_1 + L_2)}{(L_1 - L_2)^3} + \frac{2S_{3,\mathbf{0},\mathbf{0}}}{(L_1 - L_2)^3} + \frac{3\phi_2 G(L_2, \mathbf{U}_{\mathrm{p},2}, \mathbf{U}_{\mathrm{c}})}{L_2} \\
b_1 &= \frac{2S_{0,\mathbf{0},\mathbf{0}}L_2^2L_1^2}{(L_1 - L_2)^3} - \frac{S_{1,\mathbf{0},\mathbf{0}}(4L_1^2 + L_1L_2 + L_2^2)L_2}{(L_1 - L_2)^3} + \frac{2S_{2,\mathbf{0},\mathbf{0}}(L_1^2 + L_1L_2 + L_2)}{(L_1 - L_2)^3} - \frac{S_{3,\mathbf{0},\mathbf{0}}(L_1 + L_2)}{(L_1 - L_2)^3} + 3\phi_1 G(L_1 \\
b_2 &= -\frac{2S_{0,\mathbf{0},\mathbf{0}}L_2^2L_1^2}{(L_1 - L_2)^3} + \frac{S_{1,\mathbf{0},\mathbf{0}}(L_1^2 + L_1L_2 + 4L_2^2)L_1}{(L_1 - L_2)^3} - \frac{2S_{2,\mathbf{0},\mathbf{0}}(L_1^2 + L_1L_2 + L_2)}{(L_1 - L_2)^3} - \frac{S_{3,\mathbf{0},\mathbf{0}}(L_1 + L_2)}{(L_1 - L_2)^3} + 3\phi_2 G(L
\end{aligned}$$

Most of these terms represent the change in solid volume fraction and particle size due to **NUCLEATION** and **COLLISIONS**

QMOM - Binary system ($N = 2$)

- This formulation is equivalent to the solution of the first four moments (with respect to particle size) if the moments are convected with their CORRECT velocity!!

$$\frac{\partial}{\partial t}\left(m_{k,0,0}\right) + \nabla\left(\mathbf{U}_{\mathrm{p}}^{k} m_{k,0,0}\right) = S_{k,0,0},$$

VELOCITY OF THE MOMENT OF ORDER k

$$\mathbf{U}_{\mathrm{p}}^{k} = \frac{\sum_{\alpha=1}^{2} \phi_{\alpha} \mathbf{U}_{\mathrm{p},\alpha} L^{k}}{m_{k,0,0}}.$$

DQMOM/QMOM - Binary system ($N = 2$)

- With both approaches we can accommodate moments of order ONE and TWO with respect to particle velocity:

$$\frac{\partial}{\partial t}\left(\varrho_{\mathrm{p}} \phi_{\alpha} \mathbf{U}_{\mathrm{p},\alpha}\right) + \nabla\left(\varrho_{\mathrm{p}} \phi_{\alpha} \mathbf{U}_{\mathrm{p},\alpha} \mathbf{U}_{\mathrm{p},\alpha}\right) = -\phi_{\alpha} \nabla p + \phi_{\alpha} \varrho_{\mathrm{p}} \mathbf{g} + \phi_{\alpha} \varepsilon \frac{3}{4} C_{D} \varrho_{\mathrm{c}} \frac{||\mathbf{U}_{\mathrm{c}} - \mathbf{U}_{\mathrm{p},\alpha}||(\mathbf{U}_{\mathrm{c}} - \mathbf{U}_{\mathrm{p},\alpha})}{L_{\alpha}} + \varrho_{\mathrm{p}} \mathbf{c}_{\alpha}^{*}$$

$$\begin{aligned}
l = 0, k_1 = 1, k_2 = 0, k_3 = 0,\\
l = 0, k_1 = 2, k_2 = 0, k_3 = 0,\\
l = 0, k_1 = 0, k_2 = 1, k_3 = 0,\\
l = 0, k_1 = 0, k_2 = 2, k_3 = 0,\\
l = 0, k_1 = 0, k_2 = 0, k_3 = 1,\\
l = 0, k_1 = 0, k_2 = 0, k_3 = 2,
\end{aligned}$$

These terms represent the change in particle momentum due to **NUCLEATION** and **COLLISIONS**

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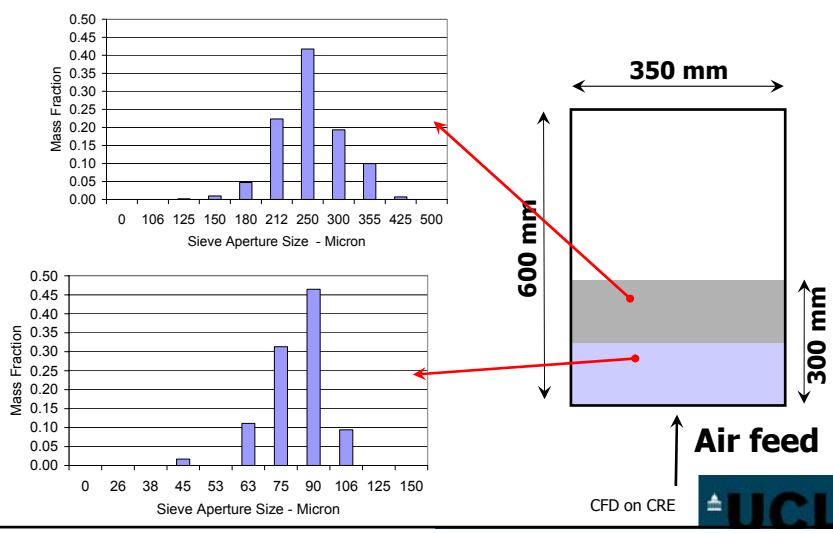
Experimental and simulation setup

- Two poly-dispersed powders were fluidized at different superficial velocities (**0.05** – **0.15** m/s)



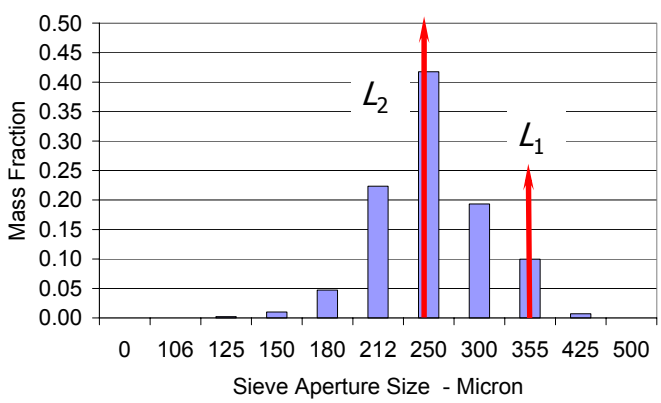
Experimental and simulation setup

- 2D simulations were run by using FLUENT 6.3
- Both DQMOM and QMOM were implemented
- The additional transport equations were implemented by using User-Defined-Subroutines (along with specific calculations for post-processing and PD algorithm)
- A very simple case was investigated (no nucleation, no aggregation, no breakage) therefore most of the source terms are null
- The drag force was calculated with the relationship developed by Mazzei & Lettieri (2006)
- The collision terms were closed by using the standard kinetic theory for granular gases

Fluid Density: 1.29E+00 kg/m^3
Fluid Viscosity: 1.85E-05 Pa s
Solid Density: 2.50E+03 kg/m^3

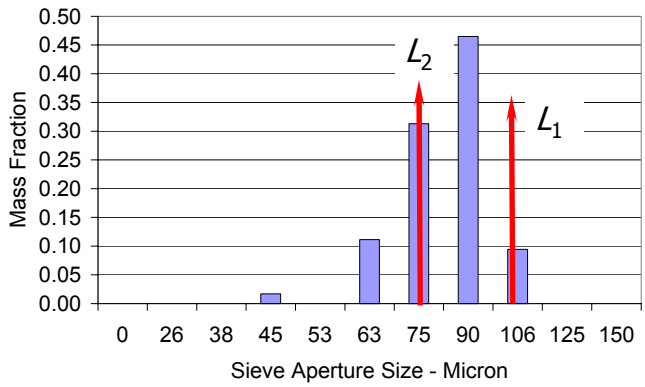
Experimental and simulation setup

- Initial conditions for particle size were calculated using the Product-Difference algorithm (TOP)



Experimental and simulation setup

- Initial conditions for particle size were calculated using the Product-Difference algorithm (BOTTOM)



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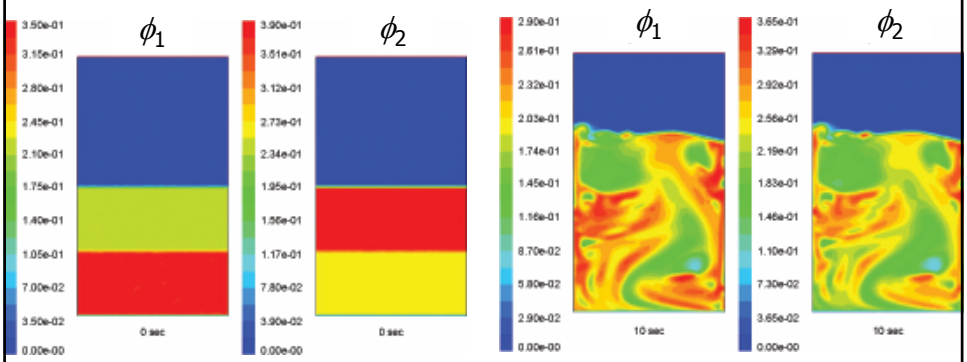
Results – simulations 0.15 m/s

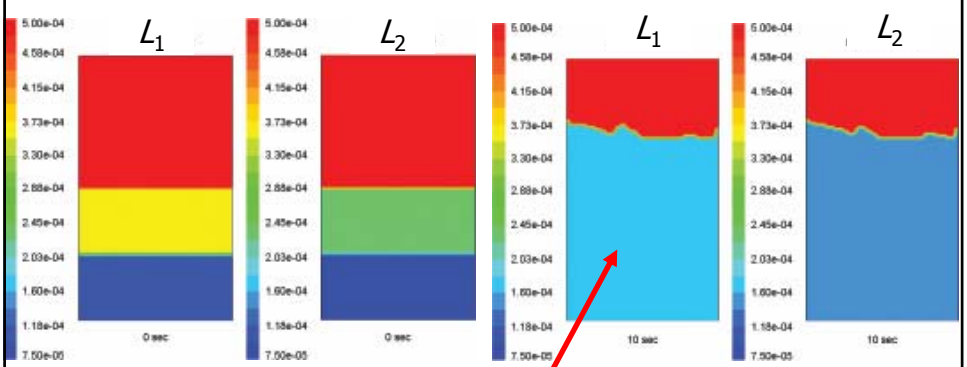
Evolution of volume fractions



$t = 0$ s $t = 10$ s

Results – simulations 0.15 m/s

Evolution of particle sizes



$t = 0$ s $t = 10$ s

FLAT CONTOUR PLOT

Results – simulations 0.15 m/s

- By manipulating the equations for the case of no nucleation, no aggregation, no breakage:

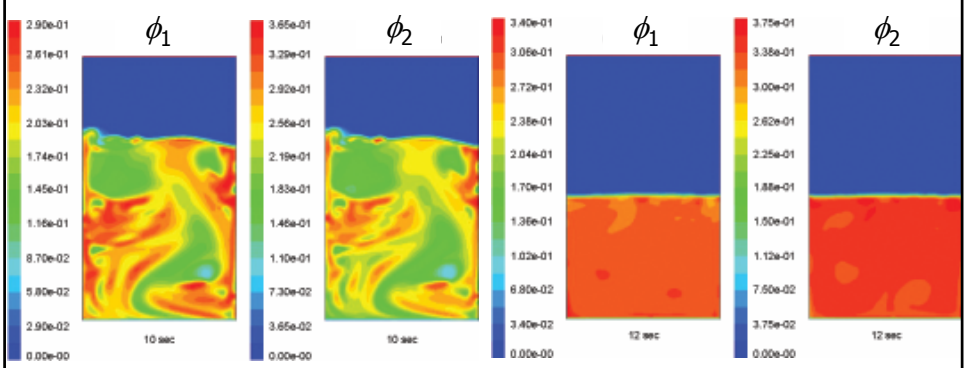
$$\frac{\partial}{\partial t}(\phi_\alpha) + \nabla(\phi_\alpha \mathbf{U}_{\mathrm{p},\alpha}) = 0$$
$$\frac{\partial}{\partial t}(\phi_\alpha L_\alpha) + \nabla(\phi_\alpha \mathbf{U}_{\mathrm{p},\alpha} L_\alpha) = 0$$

$$\Rightarrow \quad \nabla(L_\alpha) = 0$$

- … it is possible to show that all gradients in L_1 and L_2 will disappear with time resulting in flat profiles even in the case of particle segregation!
- Only if some intrinsic particle phenomena occur gradients in particle size will persist

Results – simulations 0.15 m/s

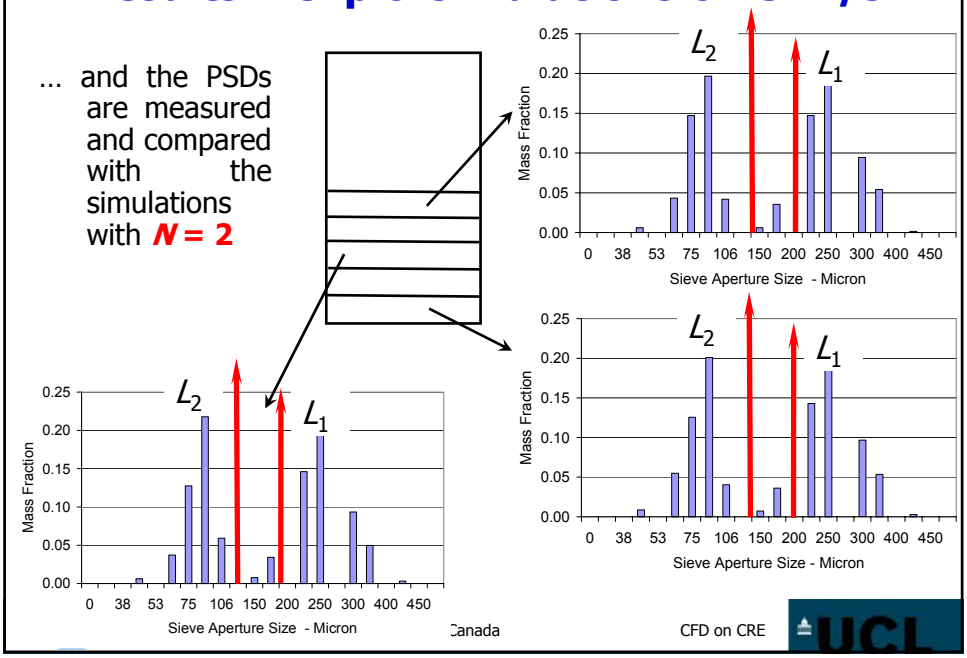
- The fluidized bed is collapsed …



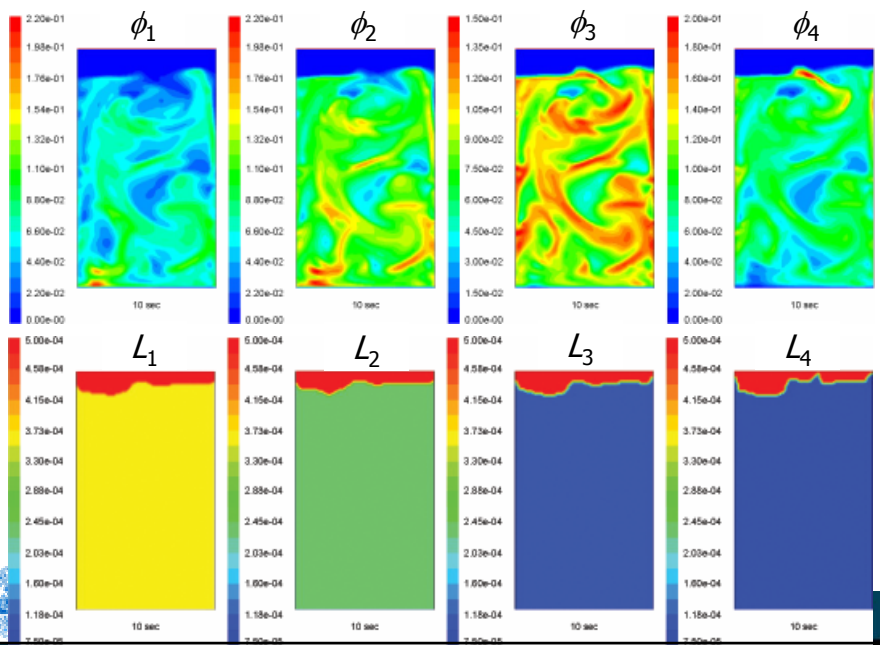
t = 10 s t = 12 s

Results – exp & simulations 0.15 m/s

… and the PSDs are measured and compared with the simulations with ***N* = 2**

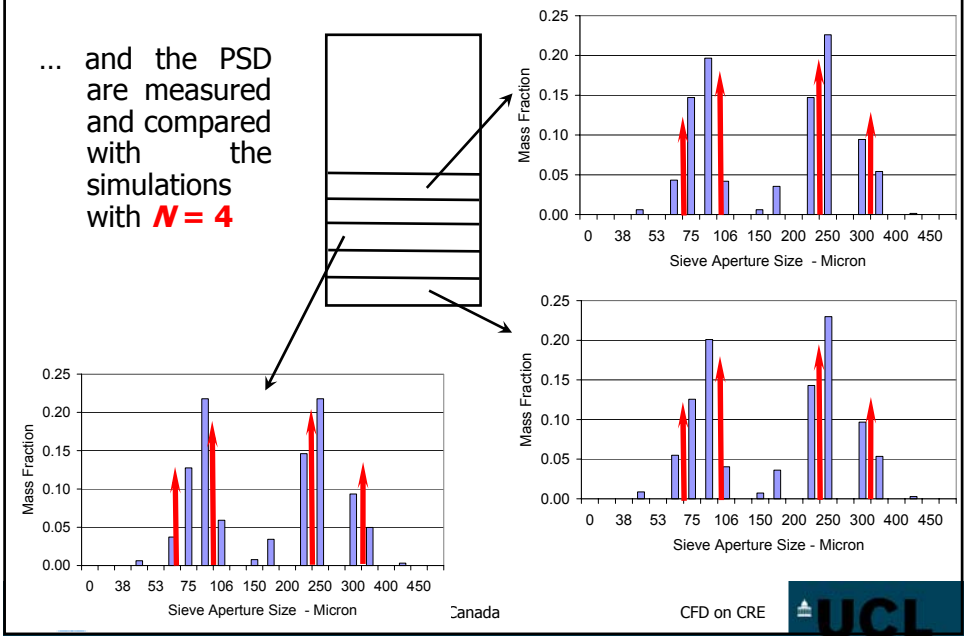


Results – simulations 0.15 m/s



Results – exp & simulations 0.15 m/s

… and the PSD are measured and compared with the simulations with ***N* = 4**



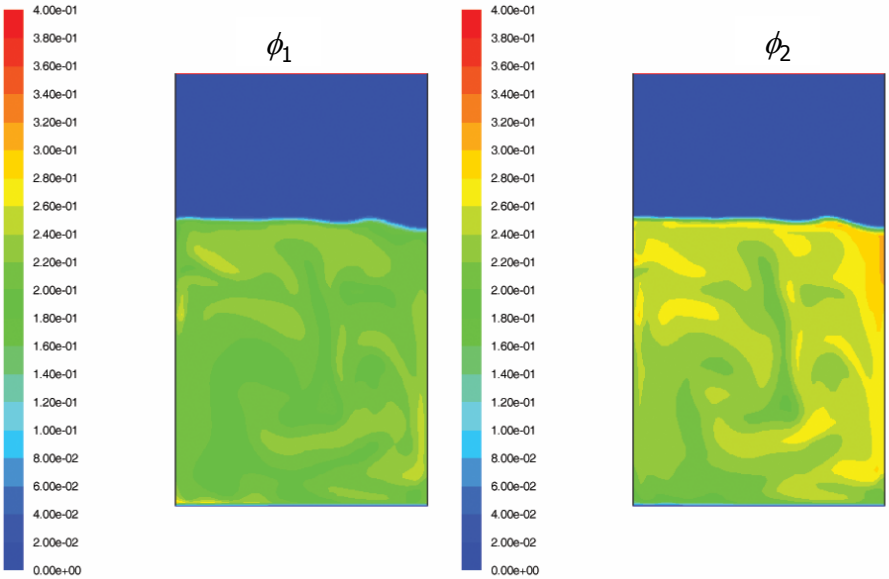
Results – exp & simulations 0.15 m/s

- Comparison between experimentally measured and simulated moments of the PSD

	Exp	***N* = 2**	***N* = 4**
M_0	0.64	0.64	0.64
M_1	1.16×10^2	0.99×10^2	1.19×10^2
M_2	2.85×10^4	1.65×10^4	2.87×10^4
M_3	7.95×10^6	2.75×10^6	8.15×10^6

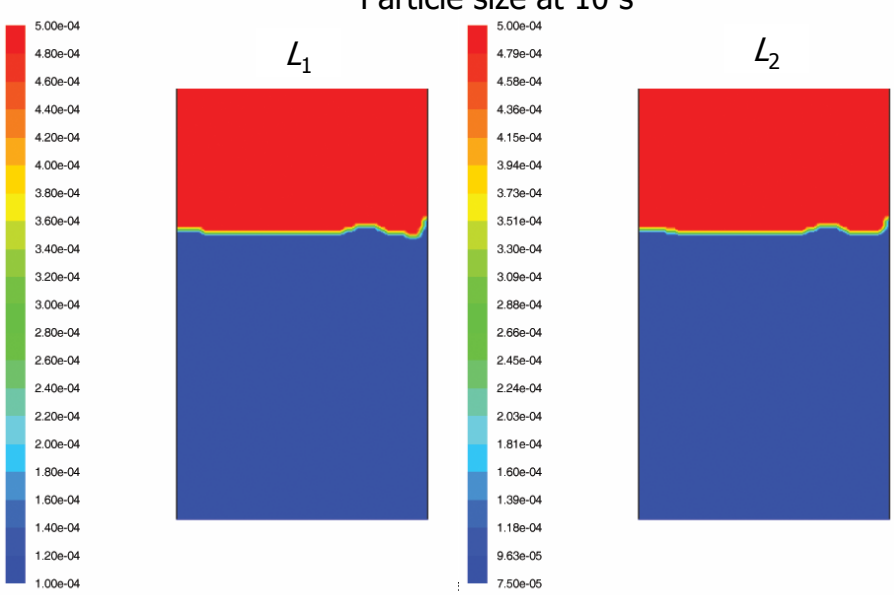
Results – simulations 0.05 m/s

Volume fractions at 10 s

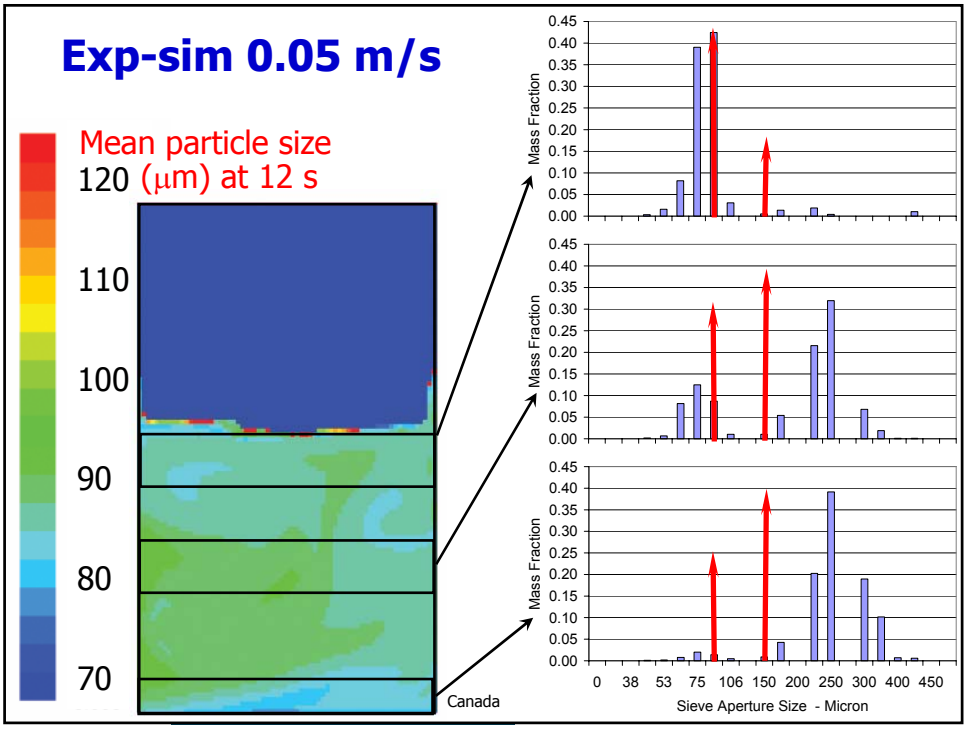


Results – simulations 0.05 m/s

Particle size at 10 s



Exp-sim 0.05 m/s



Results – exp & simulations 0.15 m/s

- Comparison between experimentally measured and simulated moments of the PSD

	TOP			BOTTOM	
	Exp.	**Sim.**		**Exp.**	**Sim.**
M_0	0.64	0.64	M_0	0.64	0.64
M_1	0.63×10^2	0.48×10^2	M_1	1.73×10^2	1.55×10^2
M_2	0.45×10^4	0.65×10^4	M_2	4.98×10^4	0.65×10^4
M_3	0.42×10^7	0.91×10^7	M_3	1.50×10^7	0.91×10^7

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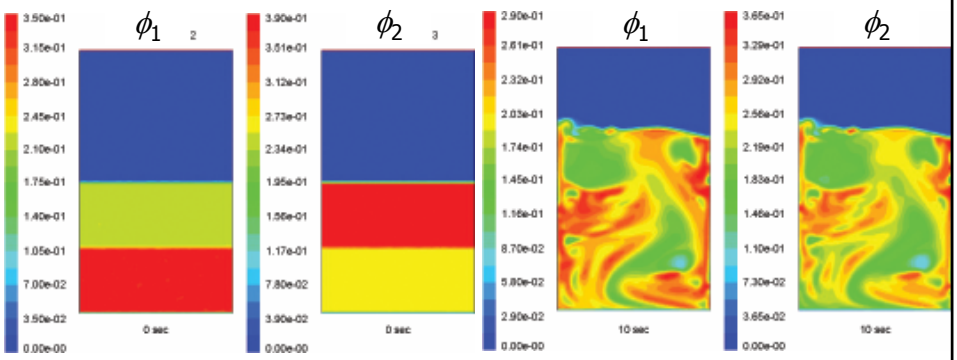
Conclusions and next steps

- From QMOM and DQMOM a new class of methods stems out (very similar to volume-averaged equations)
- QMOM and DQMOM methods are equivalent (**also in the high Stokes number limit**)
- **What is different from standards methods?** The sizes of the different particle classes are not fixed but can freely move in the particle size space
- Mixing and segregation patterns are decently predicted
- Increasing the number of nodes better and better agreement is found
- The quadrature approximation could be further exploited to solve the collision integral (integration with the kinetic theory)

Conclusions and next steps

- A few issues still need to be addressed …

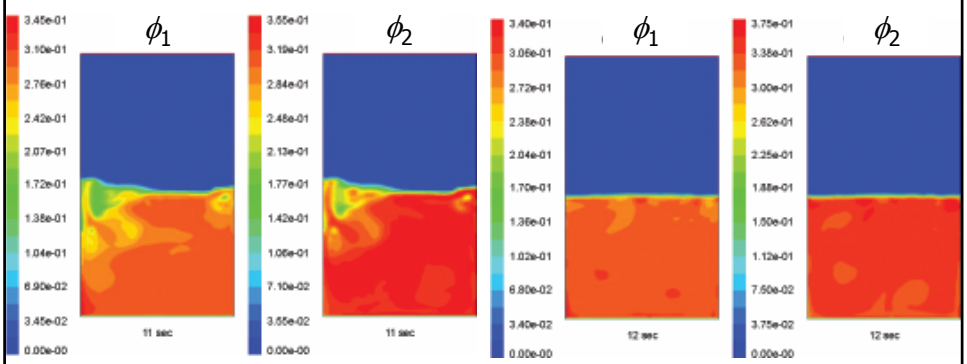


$t = 0$ s

$t = 10$ s

Conclusions and next steps

- A few issues still need to be addressed …

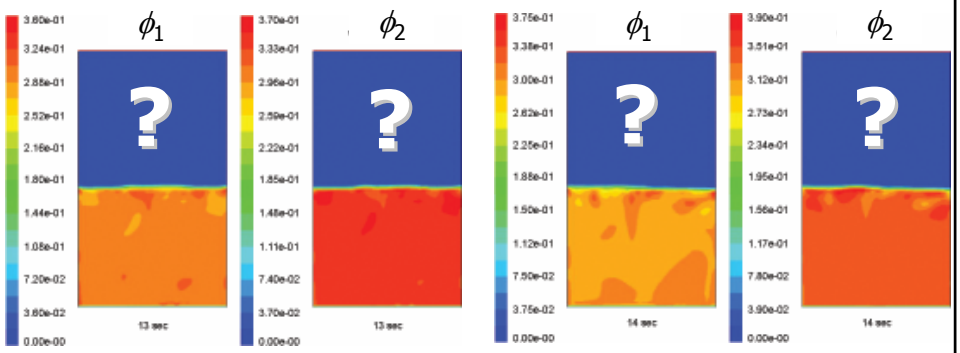


$t = 11$ s

$t = 12$ s

Conclusions and next steps

- A few issues still need to be addressed …

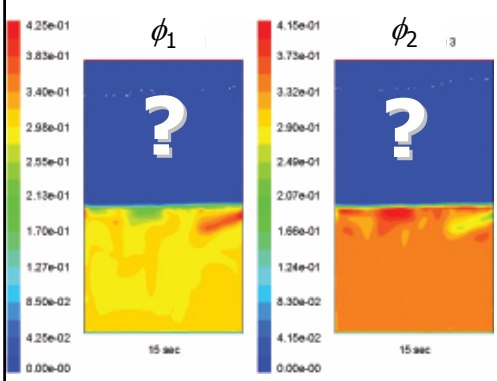


t = 13 s

t = 14 s

Conclusions and next steps

- A few issues still need to be addressed …



t = 15 s

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