Finite Size Domain Complete Set of Trial Functions Method of Moments (FCMOM) Approach in Solving PBE-CFD for Poly-disperse Flows

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NETL 2013 Conference on Multiphase Flow Science

Polydisperse Flows

Poly dispersity or distributed properties such as size and density of particles, droplets bubbles and cells occurs in significant number of chemical and biological processes. In this research , numerical simulation of the following two cases was studies:

Case 1:

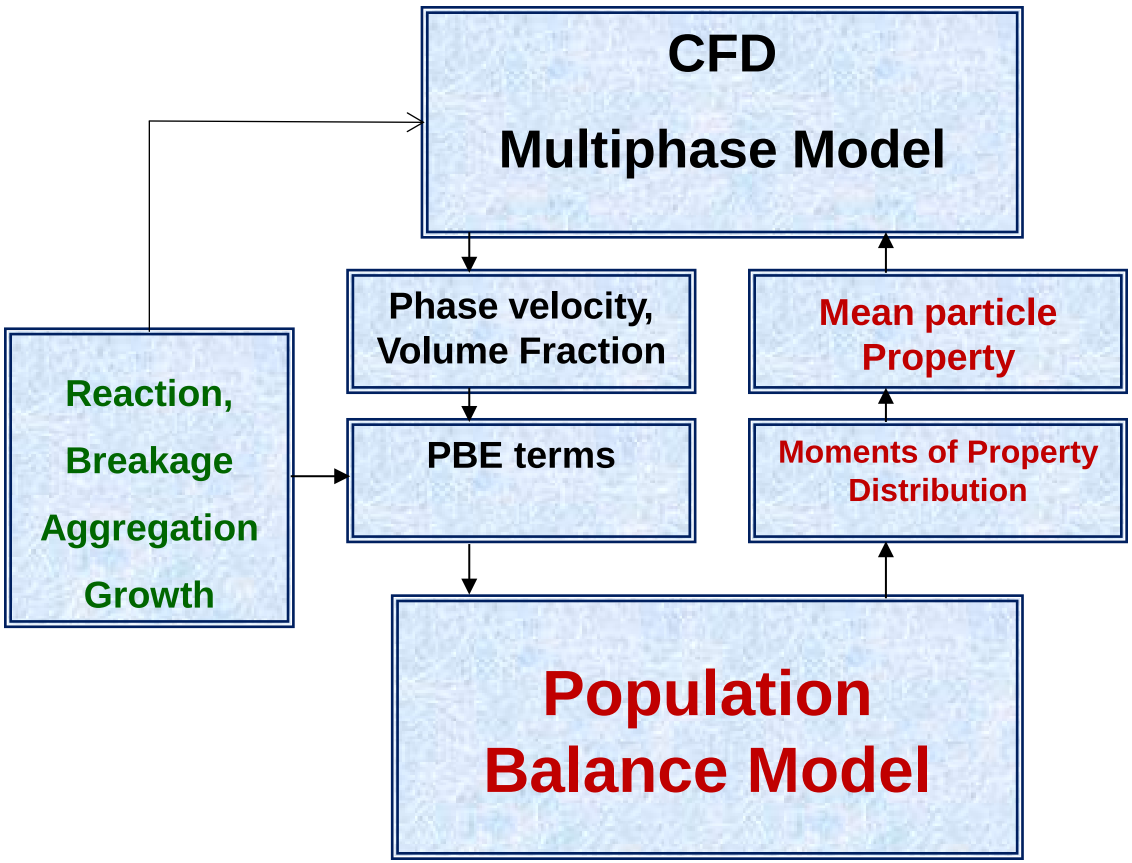
Growth Problem with No Diffusion (Application of FCMOM in Solid Phase Density Variation in a Reactive Riser Flow)

Case 2

Inhomogeneous Particle Aggregation (Coalescence of water droplets in an oil-water emulsion , and Numerical verification against QMOM model)

Population balances describes temporal and spatial evolution of the distributed properties.

Coupled CFD –Population Balance Model



Ref: Abbasi and Arastoopour, 2012, 2013

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Definitions

Postulate: Number density function $f\,(\xi;\,\mathbf{x},\,t)$

- External Coordinate $(\mathbf{x})$

  spatial position of the particle.

- Internal Coordinate (ξ)

  particle property (i.e. particle size, density, temperature,…)

What is the Population Balance Equation?

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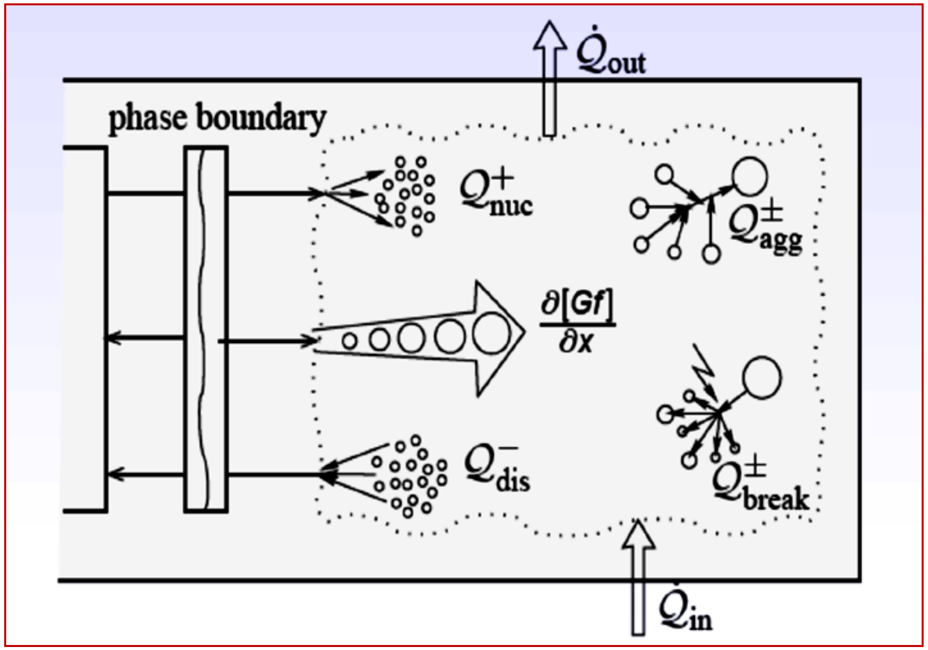


Particulate processes leading to size change:

- **Nucleation**: Produces new particles, coupled to local solubility and properties of continues phase.
- **Growth**: Mass transfer to surface of existing particles, couples to local properties of continues phase.
- **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.

$$\frac{\partial f(\xi;\mathbf{x},t)}{\partial t} + \frac{\partial}{\partial x_i}[u_p(t,\mathbf{x}) f(\xi;\mathbf{x},t)] + \frac{\partial}{\partial x_i}[D_{pt}(\xi;\mathbf{x},t)\frac{\partial f(\xi;\mathbf{x},t)}{\partial x_i}] + \frac{\partial}{\partial \xi_j}[\frac{\partial \xi_j}{\partial t} f(\xi;\mathbf{x},t)] = h(\xi;\mathbf{x},t)$$

Accumulation term + Convection term + diffusive term + Growth term = Integral Source term

Integro-Partial Differential Equation + **Closure Problem !**

FCMOM

Finite size domain Complete set of trial functions Method Of Moments: FCMOM

- Finite size domain: [-1, 1] instead of [0,∞]

$$\bar{\xi} = \frac{\{\xi - [\xi_{\min}(t) + \xi_{\max}(t)]/2\}}{[\xi_{\min}(t) + \xi_{\max}(t)]/2}$$

- Solution in terms of both Moments and size distribution
- $f(\xi,x,t)$ will be approximated by expansion based on a complete set of trial functions

$$f(\xi,x,t) = \sum_{n=0}^{\infty} C_n(t,x).\Phi_n(\xi) \qquad \text{when}$$

$$c_n = \sqrt{\frac{2n+1}{2}}.\frac{1}{2^n}.\sum_{v=0}^{n}(-1)^{n-v}.\frac{(2v)!}{[(2v-n)!]}.\{\frac{1}{[(n-v)!].[(v)!]}\}.\mu_{2v-n}$$

$$\mu_i = \int_{-1}^{1} \bar{f}'.(\bar{\xi})^i.d\bar{\xi} \qquad \phi_n(\bar{\xi}) = \sqrt{\frac{2n+1}{2}}.P_n(\bar{\xi})$$

Ref: Strumendo, Arastoopour, 2008

Case 1
Growth Problem with No Diffusion

Case 1
Growth Problem with No Diffusion

$$\frac{\partial f(\xi;\mathbf{x},t)}{\partial t}+\frac{\partial}{\partial x_i}[v_p(t,\mathbf{x})\,f(\xi;\mathbf{x},t)]+\frac{\partial}{\partial \xi_j}[\frac{\partial \xi_j}{\partial t}\,f(\xi;\mathbf{x},t)]=0 \qquad \frac{\partial \xi_j}{\partial t}=G$$

FCMOM

$$\frac{\partial \mu_i}{\partial t}+\nabla.(\mu_i.v_p)=-(MB+MB_{Conv}+IG)$$

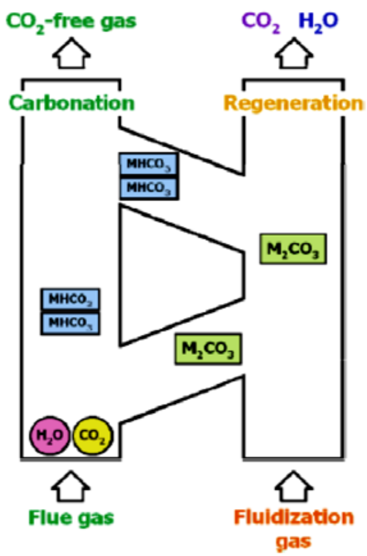
MB and MB$_{Conv}$ *: Terms due to coordinate transformation (**Moving Boundary**)*

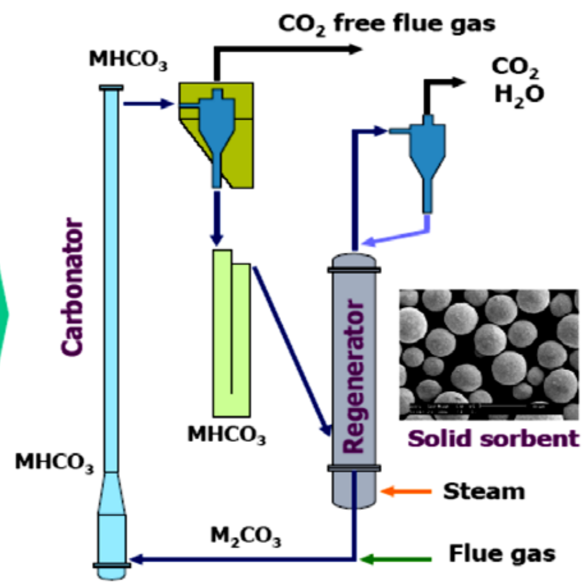
IG*: Contribution due to the* ***Integration*** *of the* ***Growth*** *Term*

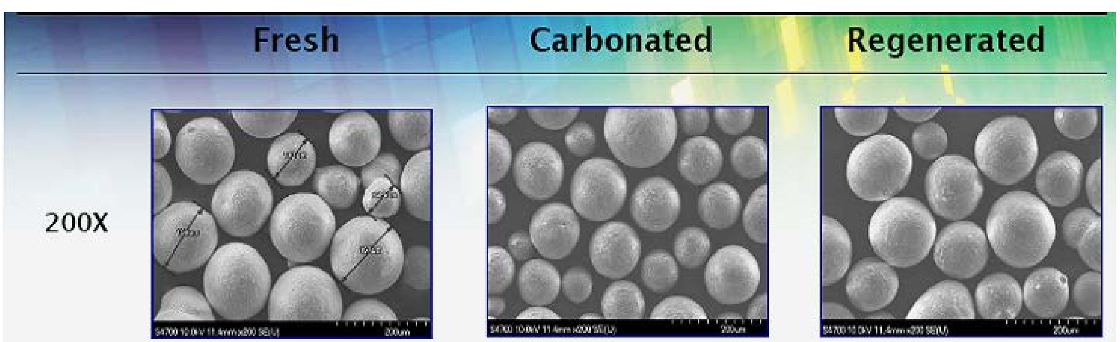
$$IG=\frac{2}{\xi_{\max}-\xi_{\min}}[(G_1.f_1-(-1)^i.G_{-1}f_{-1}]-i.\int_{-1}^{1}G.f.(\bar{v})^{i-1}d\bar{v}$$

Moving Boundary conditions: $\frac{D\bar{\xi}_{\min}}{Dt}=S_{\min}$ **and** $\frac{D\bar{\xi}_{\max}}{Dt}=S_{\max}$

Application of FCMOM in Solid Phase Density Variation in a Reactive Riser Flow

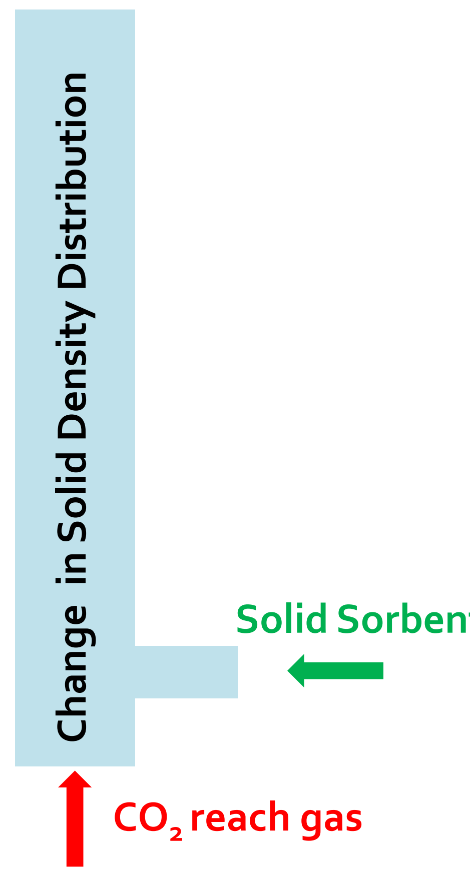






Carbonation of Metal Carbonates

$CO_2 + H_2O + M_2CO_3 \rightarrow 2MHCO_3 + Heat$



Yi et al., *International journal of greenhouse gas control*, 2007.

Governing Equation:
Constant Density Growth (Reaction) and convection

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$$\frac{\partial \mu_i}{\partial t} + \frac{\partial}{\partial x_j}[v_{p,j}\mu_i] = -\ \{[\overline{f'_{+1}} - (-1)^i.\overline{f'_{-1}}] - i.\mu_{i-1}\}.\frac{1}{(\xi_{\max} - \xi_{\min})}.(\frac{d\xi_{\min}}{dt}) -$$

$$\{[\overline{f'_{+1}} - (-1)^{i+1}.\overline{f'_{-1}}] - (i+1).\mu_i\}.\frac{1}{(\xi_{\max} - \xi_{\min})}.(-\frac{d\xi_{\min}}{dt}) -$$

$$\{[\overline{f'_{+1}} - (-1)^i.\overline{f'_{-1}}] - i.\mu_{i-1}\}.\frac{v_{p,j}}{(\xi_{\max} - \xi_{\min})}.(\frac{\partial\xi_{\min}}{\partial x_j}) -$$

$$\{[\overline{f'_{+1}} - (-1)^{i+1}.\overline{f'_{-1}}] - (i+1).\mu_i\}.\frac{v_{p,j}}{(\xi_{\max} - \xi_{\min})}.(-\frac{\partial\xi_{\min}}{\partial x_j})$$

Lower Boundary (Fresh Sorbent Density) is a Moving Boundary

$$\frac{\partial \xi_{\min}}{\partial t} + v_p.\nabla\xi_{\min} = K$$

$$\frac{\partial \xi_{\max}}{\partial t} = 0$$

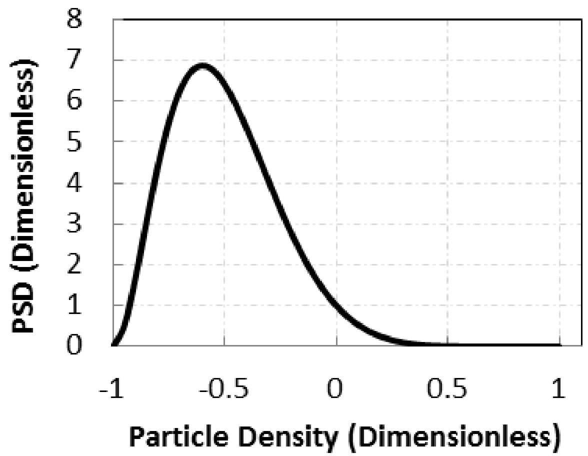
Mean Density

$$\rho_s = \frac{(\frac{\mu_1}{\mu_0})(\xi_{\max} - \xi_{\min}) + (\xi_{\min} + \xi_{\max})}{2}$$

Boundary Conditions

- Gas inlet velocity
  - 0.5 m/s
- Solid Inlet Velocity
  - 0.15 m/s
- Outlet pressure
  - 1 atm
- Moments inlet values

Dimensionless Inlet distribution

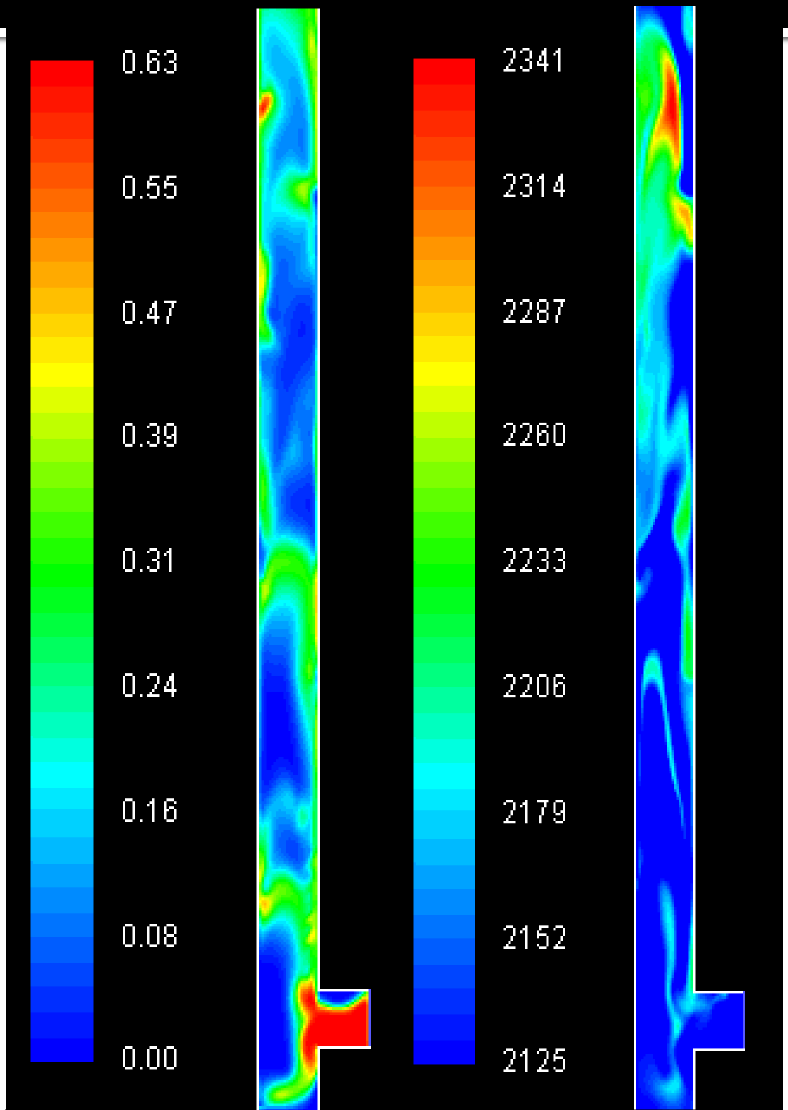


Minimum Density
2000 kg/m^3

Maximum Density
2500 kg/m^3

Mean Density
2125 kg/m^3

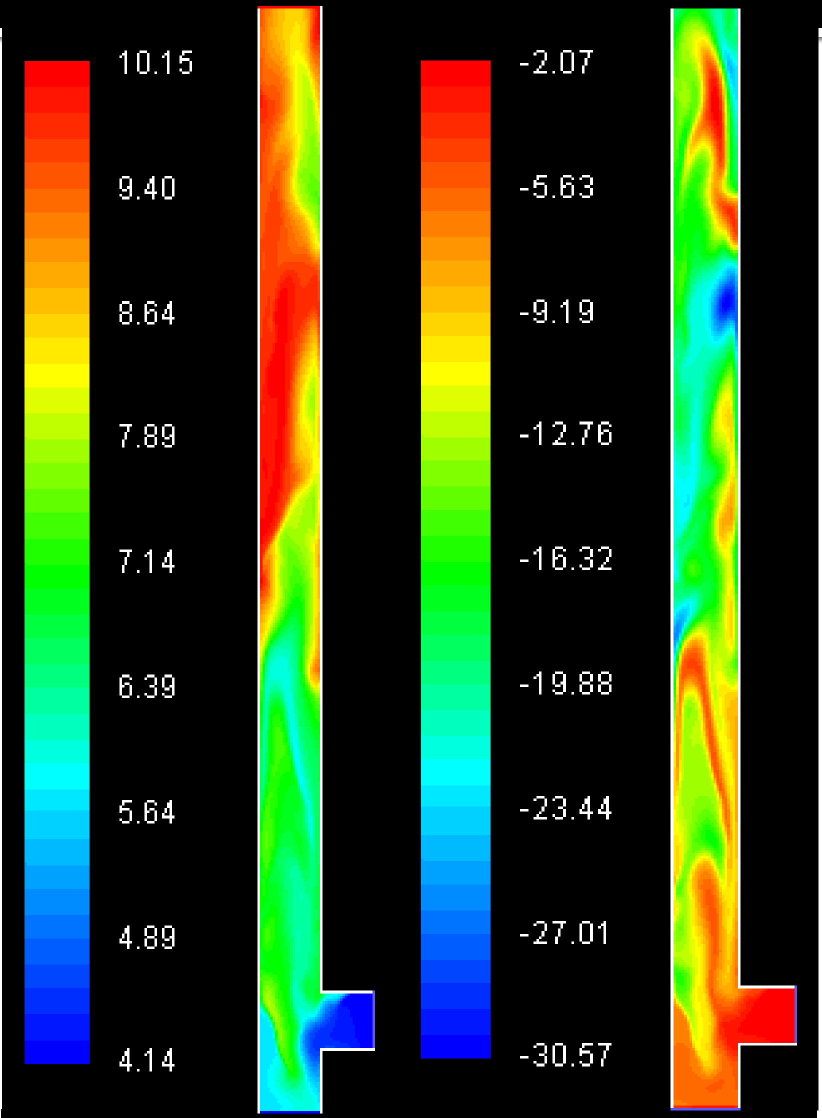
Results at *t*= 5 *sec* with an Arbitrary constant Reaction Rate



Solid Volume Fraction

Mean Solid Density

Results at *t= 5 sec* with an Arbitrary constant Reaction Rate



1st moment of distribution

2nd moment of distribution

Case 2
Inhomogeneous Particle Aggregation

Coalescence of water droplets in an oil-water emulsion , and Numerical verification against QMOM model

Homogeneous Particle Aggregation

- Continuous Smoluchowski Equation (CSE)

$$\frac{\partial f(v;\mathbf{x},t)}{\partial t} = \frac{1}{2}\int_0^v \beta(v-\eta,\eta).f(v-\eta,t).f(\eta,t)d\eta - f(v,t).\int_0^\infty \beta(v,\eta).f(\eta,t)d\eta$$

- Finite Smoluchowski Equation (FSE)

$$\frac{\partial f(v;\mathbf{x},t)}{\partial t} = \frac{1}{2}H(v-2v_{\min})\int_{v_{\min}}^{v-v_{\min}} \beta(v-\eta,\eta).f(v-\eta,t).f(\eta,t)d\eta$$
$$- f(v,t).H[(v_{\max}-v_{\min})-v].\int_{v_{\min}}^{v_{\max}-v} \beta(v,\eta).f(\eta,t)d\eta$$

  - v_{min} and v_{max} are set initially.
  - Introducing Heaviside step function, aggregations leading to particles greater than v_{max} are neglected.
  - For $v_{min}=0$ and large enough v_{max} solution of FSE converges to CSE.

Ref: Strumendo, Arastoopour, 2008

Inhomogeneous Particle Aggregation

$$\frac{\partial f(v;\mathbf{x},t)}{\partial t}+\frac{\partial}{\partial x_i}[u_p(t,\mathbf{x})\,f(v;\mathbf{x},t)]=\frac{1}{2}H(v-2v_{\min})\int_{v_{\min}}^{v-v_{\min}}\beta(v-\eta,\eta).f(v-\eta,t).f(\eta,t)d\eta$$

$$-\,f(v,t).H[(v_{\max}-v_{\min})-v].\int_{v_{\min}}^{v_{\max}-v}\beta(v,\eta).f(\eta,t)d\eta$$

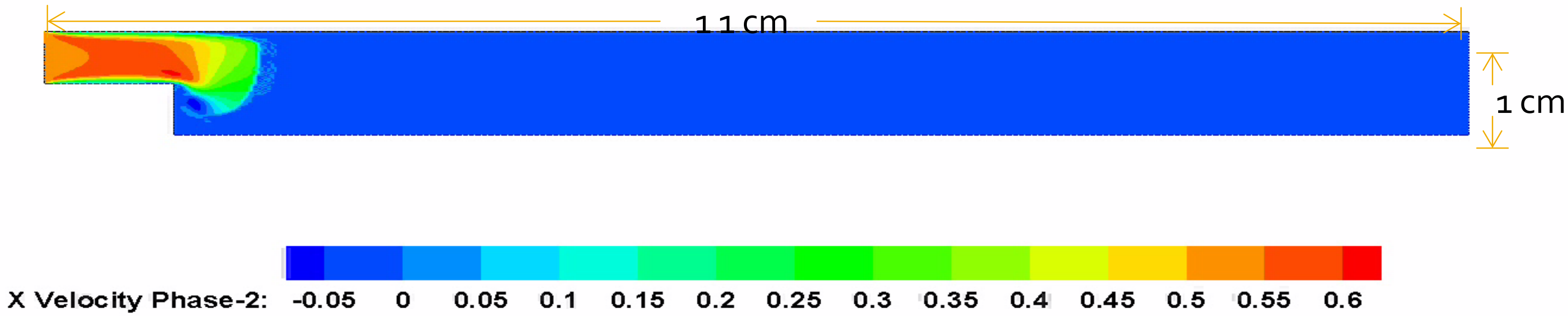
FCMOM

$$\frac{\partial\mu_i}{\partial t}+\nabla.(\mu_i.v_p)=\frac{v_{\max}-v_{\min}}{4}\sum_{n=0}^{M-1}\sum_{m=0}^{M-1}c_m c_n E_{mni}^{FSE}-\frac{v_{\max}-v_{\min}}{2}\sum_{n=0}^{M-1}\sum_{m=0}^{M-1}c_m c_n F_{mni}^{FSE}$$

$$E_{mni}^{FSE}=\int_{-2+v_r}^{1}\int_{-1}^{\bar{v}+1-v_r}\bar{v}^i\beta\left[\frac{v_{\max}-v_{\min}}{4}.(\bar{v}-\bar{\eta}),\frac{v_{\max}-v_{\min}}{4}.(\bar{\eta}-v_r)\right]\phi_m(\bar{v}-\bar{\eta}-v_r)\phi_n(\bar{\eta})d\bar{\eta}d\bar{v}$$

$$F_{mni}^{FSE}=\int_{-2+v_r}^{2-v_r}\int_{-1}^{1-\bar{v}-v_r}\bar{v}^i\phi_m(\bar{v}).\beta\left[\frac{v_{\max}-v_{\min}}{4}.(\bar{v}+v_r),\frac{v_{\max}-v_{\min}}{4}.(\bar{\eta}+v_r)\right]\phi_n(\bar{\eta})d\bar{\eta}d\bar{v}$$

Coalescence of water droplets in an oil-water emulsion in BFS



Water in Oil Emulsion

Inlet condition: 5% water content Re= 500 d10= 12.5 μm

inlet size distribution: $f(\bar{v},0) = a.(\frac{1}{2}+\frac{\bar{v}}{2})^q.(\frac{1}{2}-\frac{\bar{v}}{2})^p$

Aggregation Kernel: $\beta(v,\eta) = \beta_o(v+\eta)$ Simulation time: 1 sec

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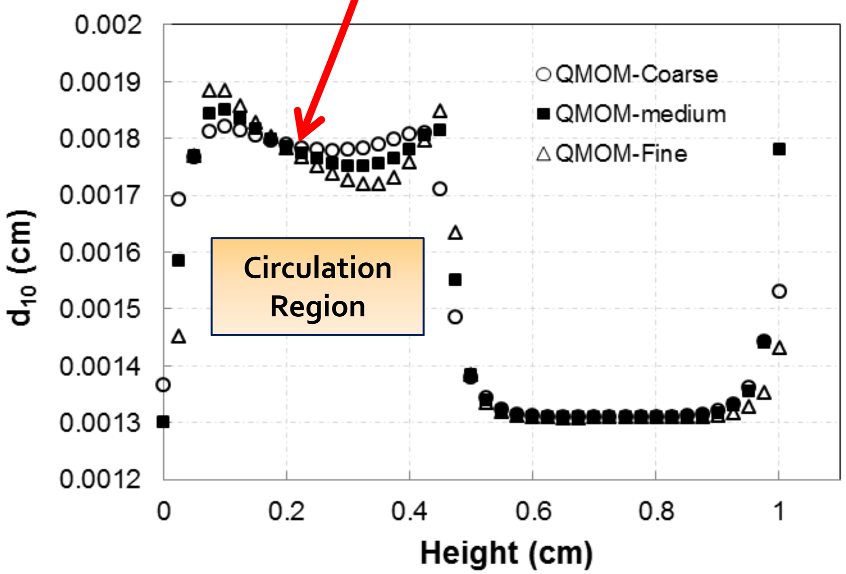
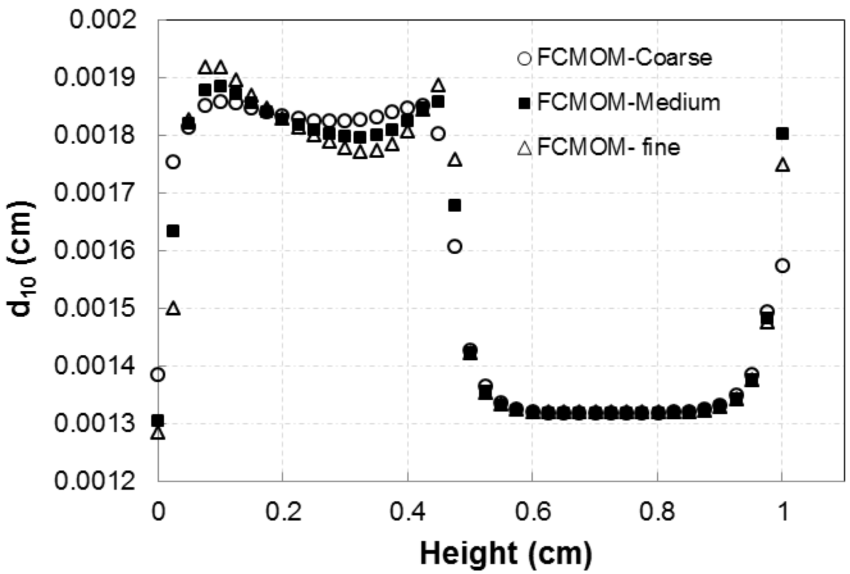
Numerical verification against QMOM model (Mesh size)

Instantaneous Mean Droplet size contours at *t= 1 sec*





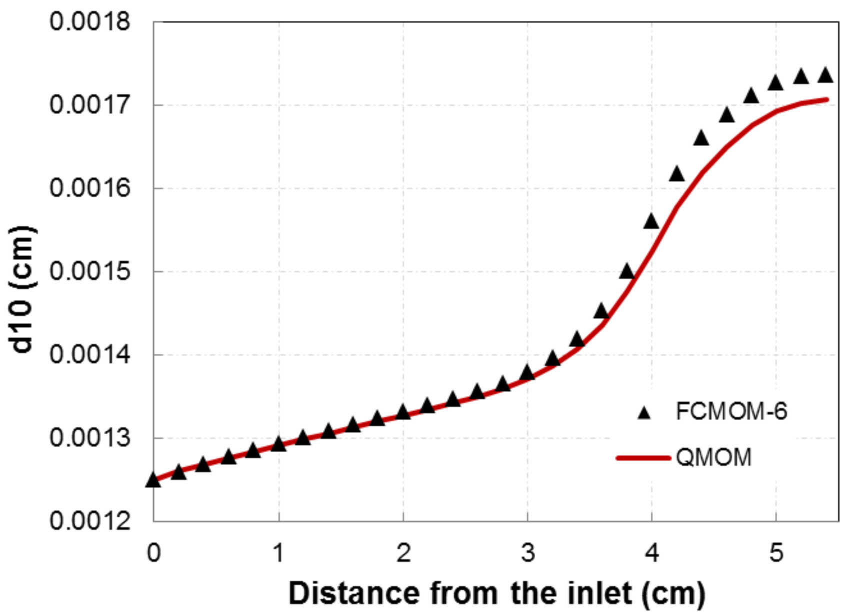
Mesh Independence

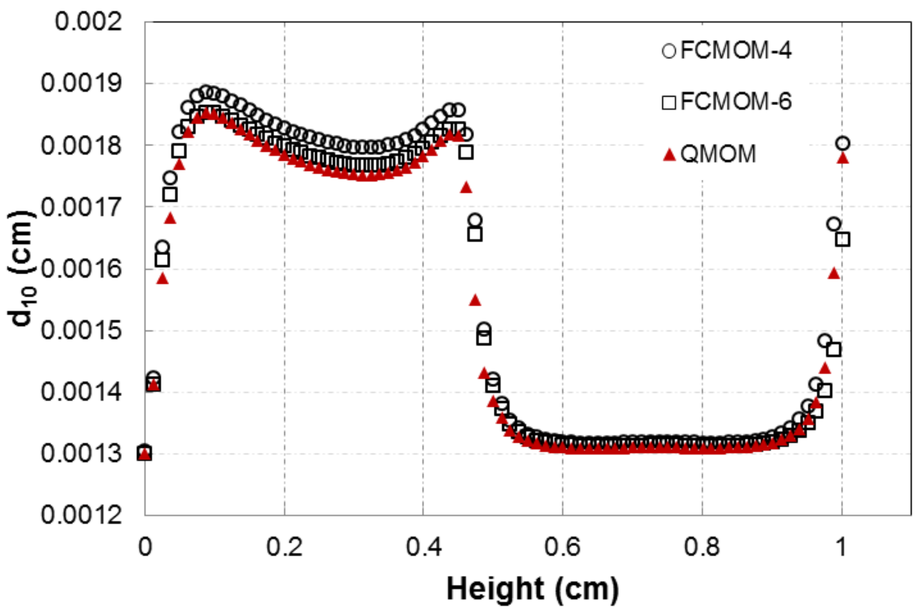
Coarse: 8400 cell

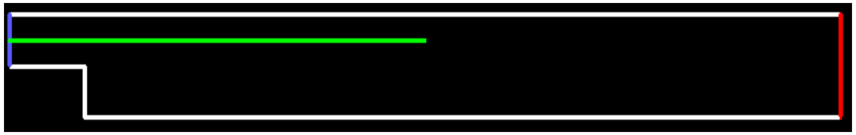
Medium: 33600 cell

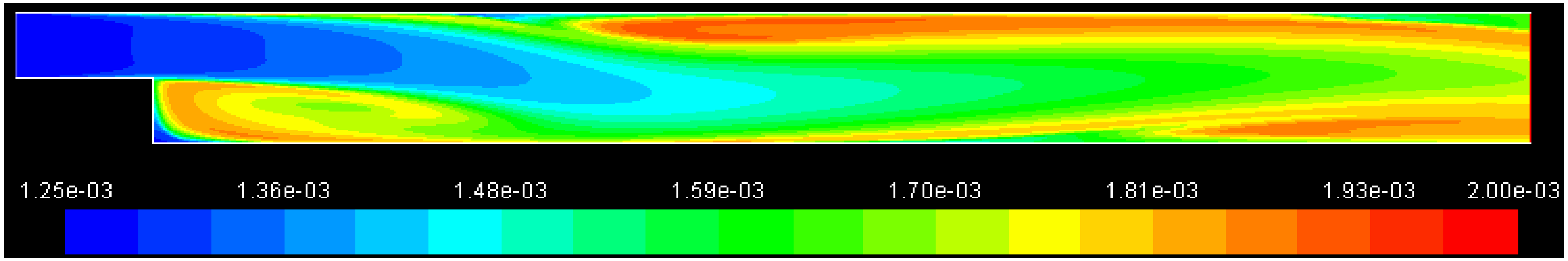
Fine: 134400 cells

Numerical verification against QMOM model (cont'd)









Concluding and Remarks

- Coupling and Implementation of FCMOM in ANSYS Fluent was successful.
- The method is fast, computationally effective and stable.
- Provides both moments and reconstructed distribution function.
- FCMOM is an excellent choice when the actual distribution is important.
- Computational time is same as QMOM for the same number of moments.

Open Issues/Future work

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- Particulate phase velocity (moments convection) is independent of internal coordinate.
- Discretization is limited to First-order schemes.
- First-order scheme introduces Numerical diffusion.
- In aggregation problems higher order moments $(i > 6)$ are not stable.
- Future work will be focused on a method to overcome the above mentioned problem.

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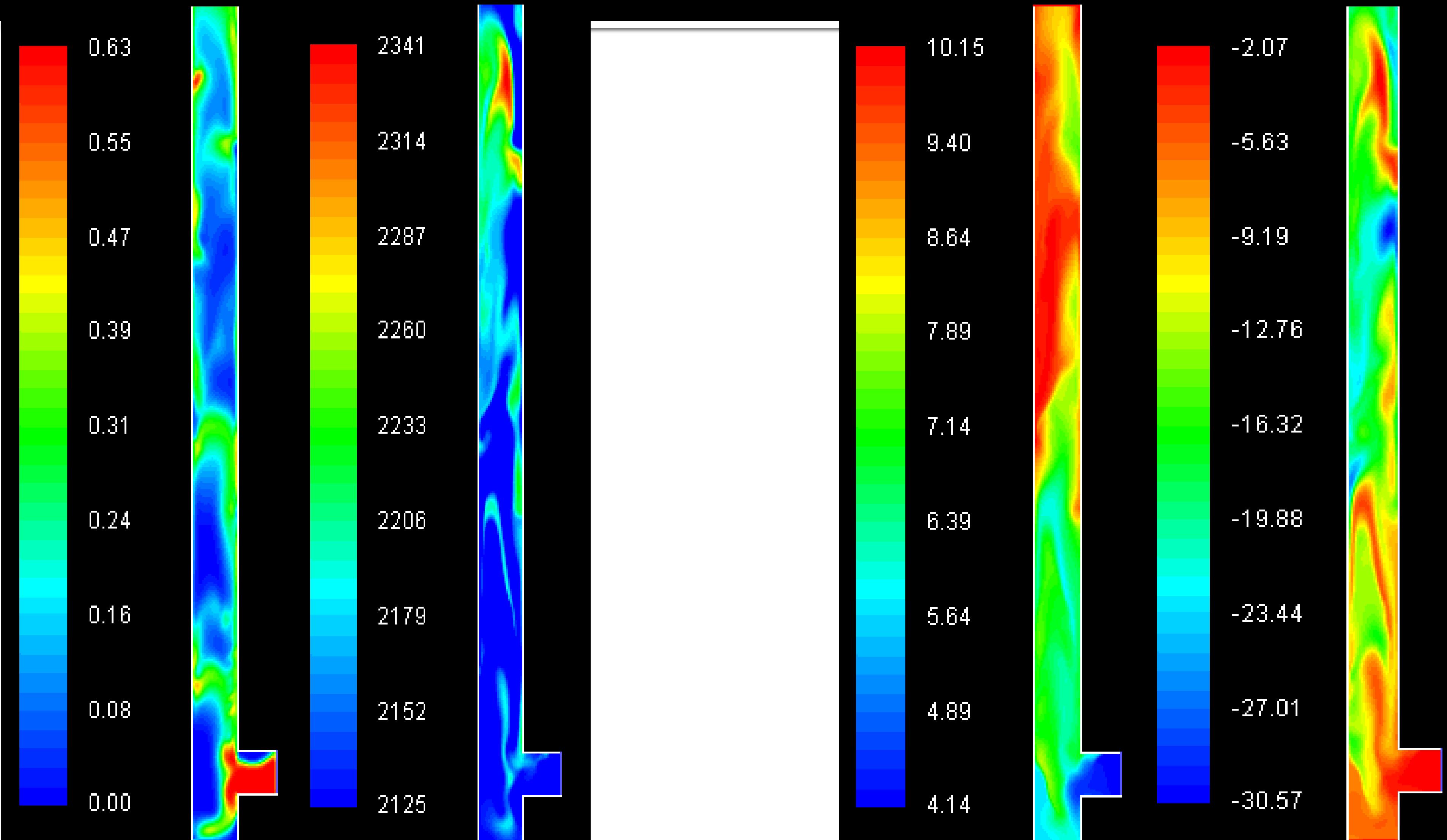
Acknowledgement

Thanks to the Department of Energy (DOE) for financial support.

Results at *t= 5 sec* with an Arbitrary constant Reaction Rate



Solid Volume Fraction

Mean Solid Density

1st moment of distribution

2nd moment of distribution