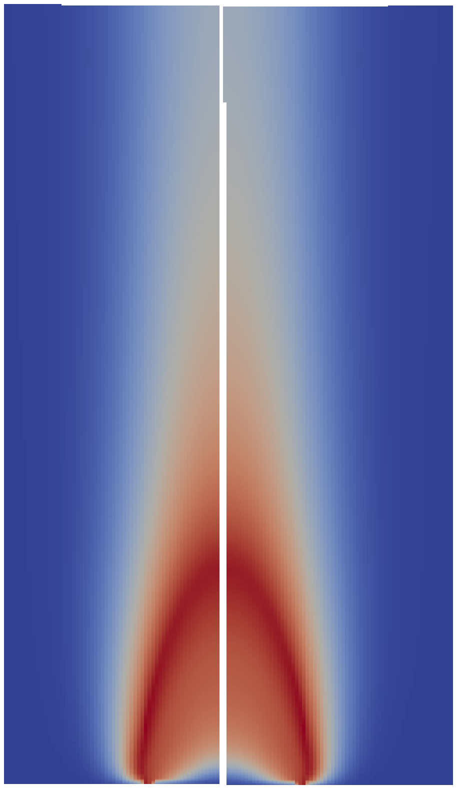
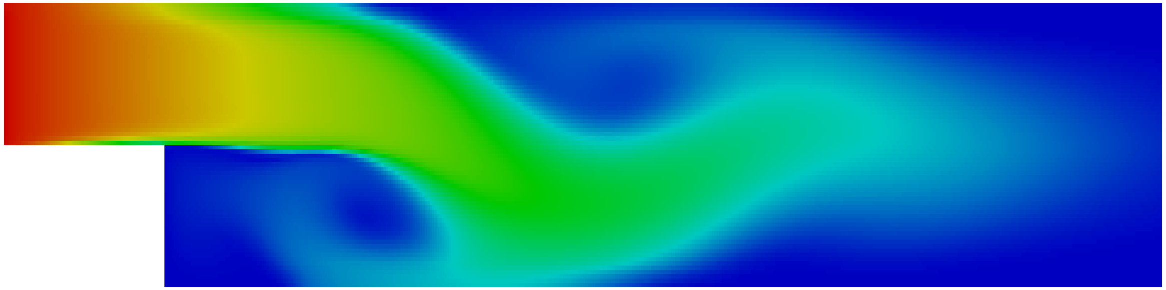
Computational Modelling of Multiphase, Turbulent, (Reactive) Flows





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CoMo (Computational Modelling) Group
Graduate Conference Presentation

30th March 2010

Contents

1) Theory
- Computational Fluid Dynamics (CFD)
- Population Balances (PBE)

2) Methods
- Quadrature Method of Moments (QMoM)
- Direct Quadrature Method of Moments (DQMoM)

3) Results
- Coupled CFD/PBE with complex closures

What to take away from this talk

Multiphase processes are encountered frequently in industry (*e.g.* gas-liquid contacting, reactors, drying).

The aim of this research is to improve multiphase flow models by coupling population balance equations (PBEs) to computational fluid dynamics (CFD) codes.

Coupling population balances to computational fluid dynamics codes can help predict trends in behaviour of multiphase flows in real equipment.

Why is this research relevant?

Multiphase processes are:

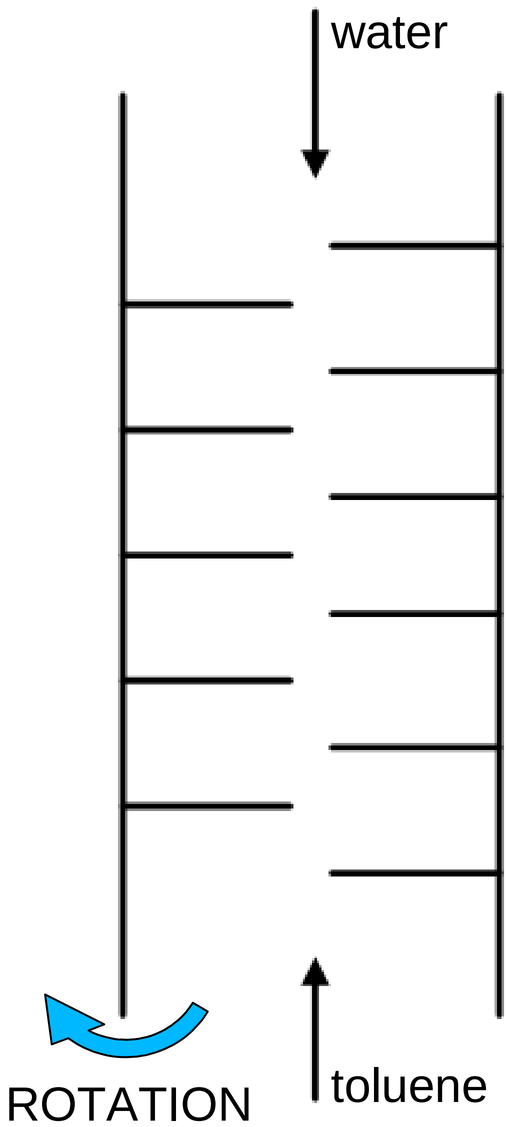
- highly complex
- challenging to solve numerically
- computational models and methods are not general

e.g. Recent TCE article on improving the efficiency of a rotating disc contactor (RDC). They used a pilot plant.

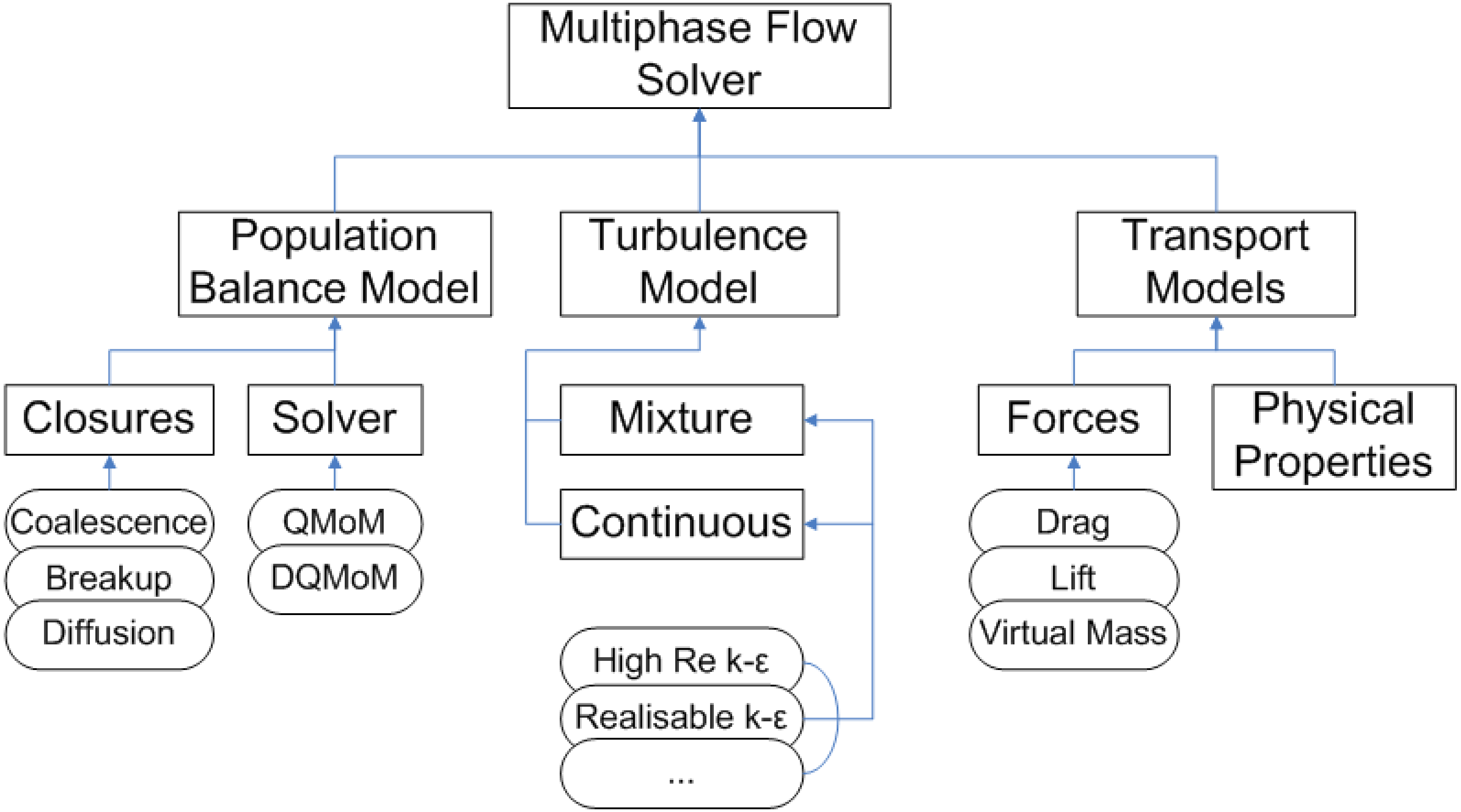
CFD is cheap, especially when it is free (OpenFOAM†)!

† http://www.openfoam.com

What problem will I solve?



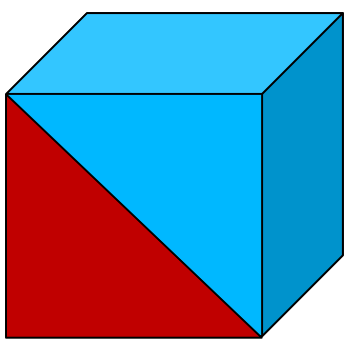
Code Design


Multiphase Flow Solver
Population Balance Model
Turbulence Model
Transport Models
Closures
Solver
Mixture
Continuous
Forces
Physical Properties
Coalescence
Breakup
Diffusion
QMoM
DQMoM
High Re k-ε
Realisable k-ε
...
Drag
Lift
Virtual Mass

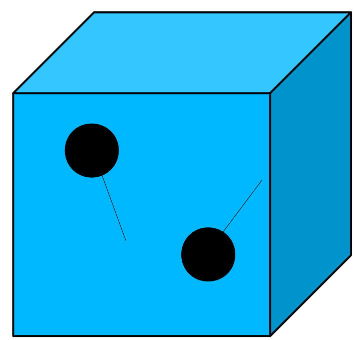
How may this problem be solved?

Increasing Scale

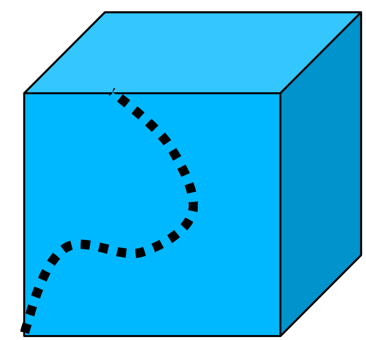
Euler/Euler



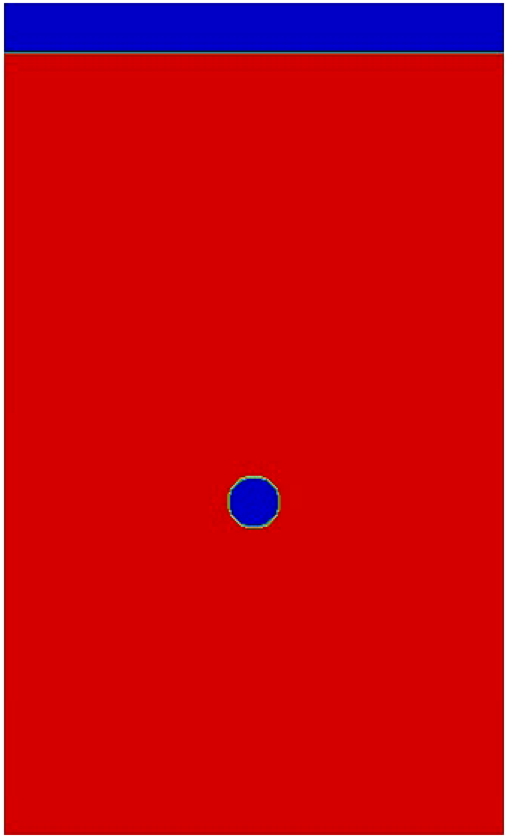
Euler/Lagrange



Volume of Fluid
Level Set



Why use a population balance?



Volume of Fluid Method:
Air bubble rising in water.

Euler/Euler – no information on the size distribution of the dispersed phase.

Droplets with different sizes will have different effects on the drag force on the continuous phase.

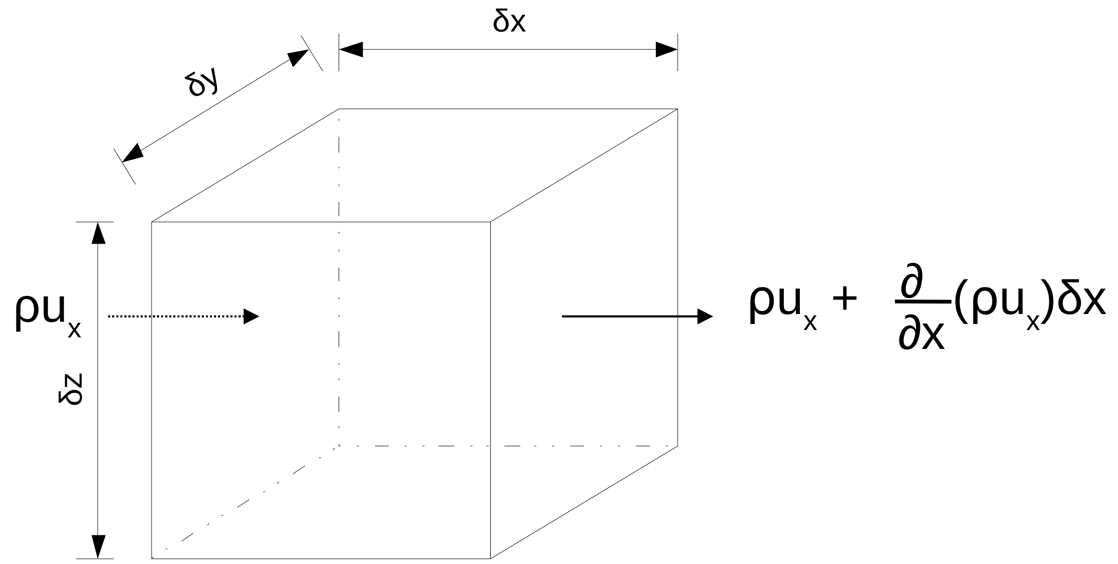
Theory

Navier-Stokes equations

The equations governing fluid flow are conceptually simple:

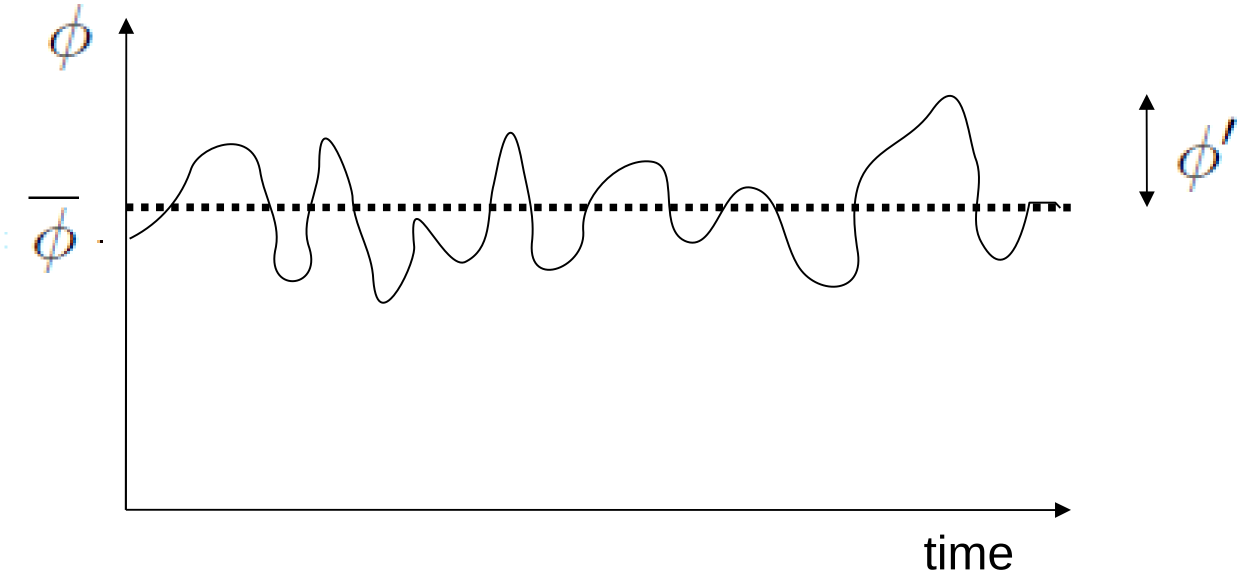
1) The mass of fluid is conserved.
2) Rate of change of momentum equals the sum of forces on a fluid element.
   Newton's 2nd Law (F = m a).

Treat the fluid as a continuum. i.e. individual molecular interactions are ignored.



Reynolds Averaging

Turbulent flows are **Random / Chaotic**



So the following substitutions are applied to the Navier-Stokes equations: $\phi = \overline{\phi} + \phi'$

Multiphase Flow – Euler/Euler

Continuity:

$$\frac{\partial \rho_\varphi \alpha_\varphi}{\partial t} + \nabla \cdot (\rho_\varphi \alpha_\varphi \boldsymbol{u}_\varphi) = 0$$

Conservative form of the momentum equation:

$$\frac{\partial \rho_\varphi \alpha_\varphi \boldsymbol{u}_\varphi}{\partial t} + \nabla \cdot (\rho_\varphi \alpha_\varphi \boldsymbol{u}_\varphi \boldsymbol{u}_\varphi)$$
$$= - \alpha_\varphi \nabla p + \nabla \cdot \left(\rho_\varphi \alpha_\varphi \mathbf{T}_\varphi^{\text{eff}}\right) + \mathbf{M}_\varphi + \rho_\varphi \alpha_\varphi \boldsymbol{g}$$

Non-Conservative form of the momentum equation:

$$\frac{\partial \boldsymbol{u}_\varphi}{\partial t} + \boldsymbol{u}_\varphi \cdot \nabla \boldsymbol{u}_\varphi$$
$$= - \frac{\nabla p}{\rho_\varphi} + \nabla \cdot \left(\mathbf{T}_\varphi^{\text{eff}}\right) + \frac{\nabla \alpha_\varphi}{\alpha_\psi} \cdot \mathbf{T}_\varphi^{\text{eff}} + \frac{\mathbf{M}_\varphi}{\rho_\varphi \alpha_\varphi} + \boldsymbol{g}$$

Drag force

Important, as this is how the coupling between CFD and PBE is achieved.

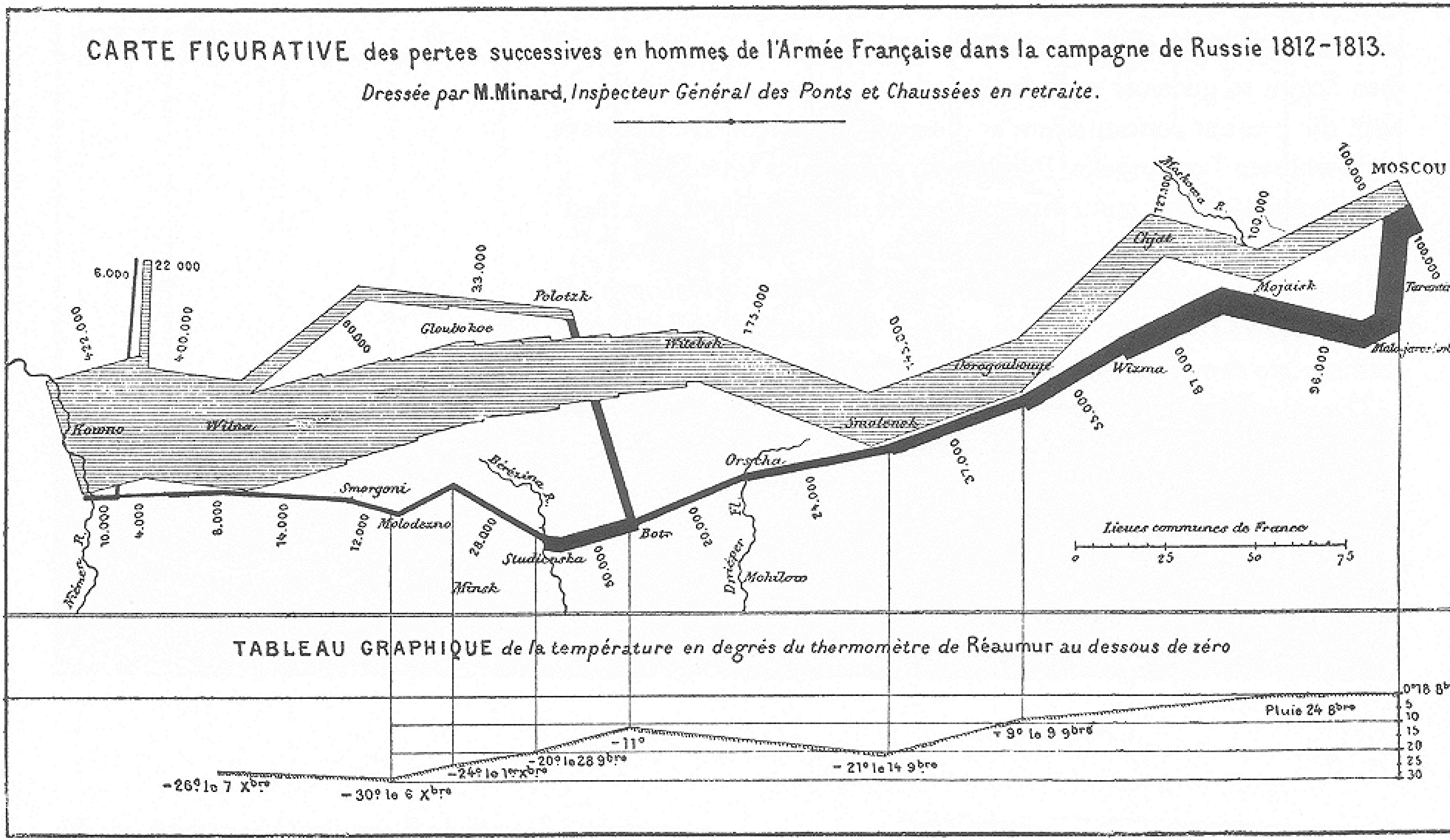
$$\mathbf{M}_{d,i} = \frac{3}{4} \frac{\rho_c \ \alpha_c \ \alpha_{di} \ C_D}{d_{32}} \left| \boldsymbol{u}_c - \boldsymbol{u}_{d,i} \right| \left(\boldsymbol{u}_c - \boldsymbol{u}_{d,i} \right)$$

$$\mathbf{M}_c = - \sum_{i=0}^{N_d} \mathbf{M}_{d,i}$$

Turbulence Modelling

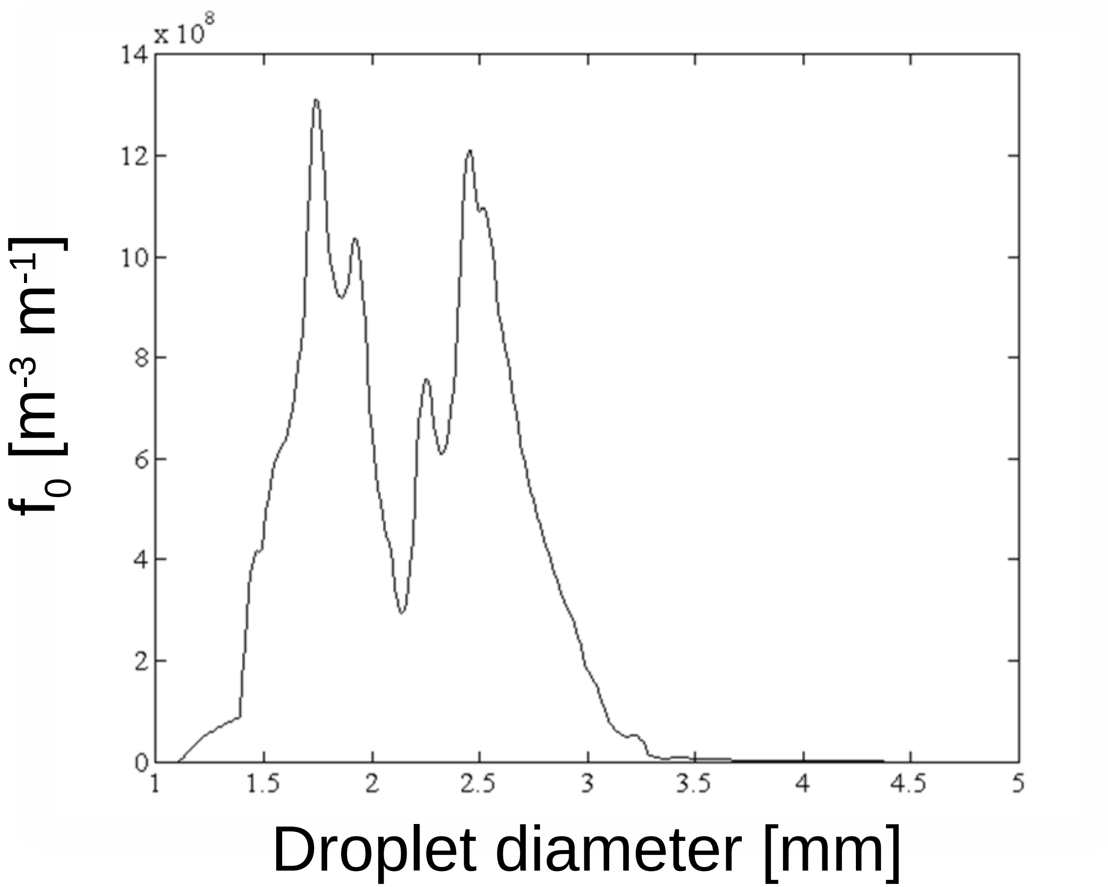
Mixture Models	- Averaged flow variables
Continuous Models	- Apply algebraic relationship to get turbulence in the dispersed phase.
Continuous & Dispersed Models	- Solve separate turbulence equations for each phase and couple them.

Theory – Population Balances



The Number Size Density

$$f_0\left(L;\ \boldsymbol{x}, t\right)$$



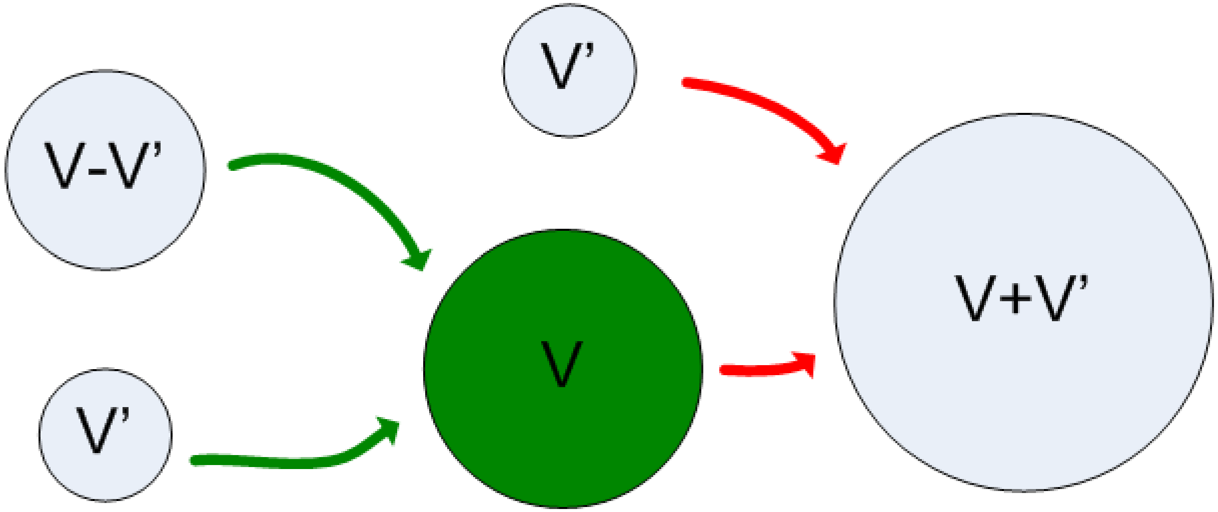
Population Balance Equation

$$\frac{\partial f_0(L)}{\partial t} + \nabla \cdot \left(\, \langle \boldsymbol{u} | L \rangle \; f_0(L) \, \right) = S(L)$$

Droplet Coalescence

$$S(V) = \frac{1}{2}\int_0^V \beta(V - V', V')\ f_0(V - V')\ f_0(V')\ dV'$$

$$- f_0(V)\int_0^\infty \beta(V, V')\ f_0(V')\ dV'$$



Coalescence Models

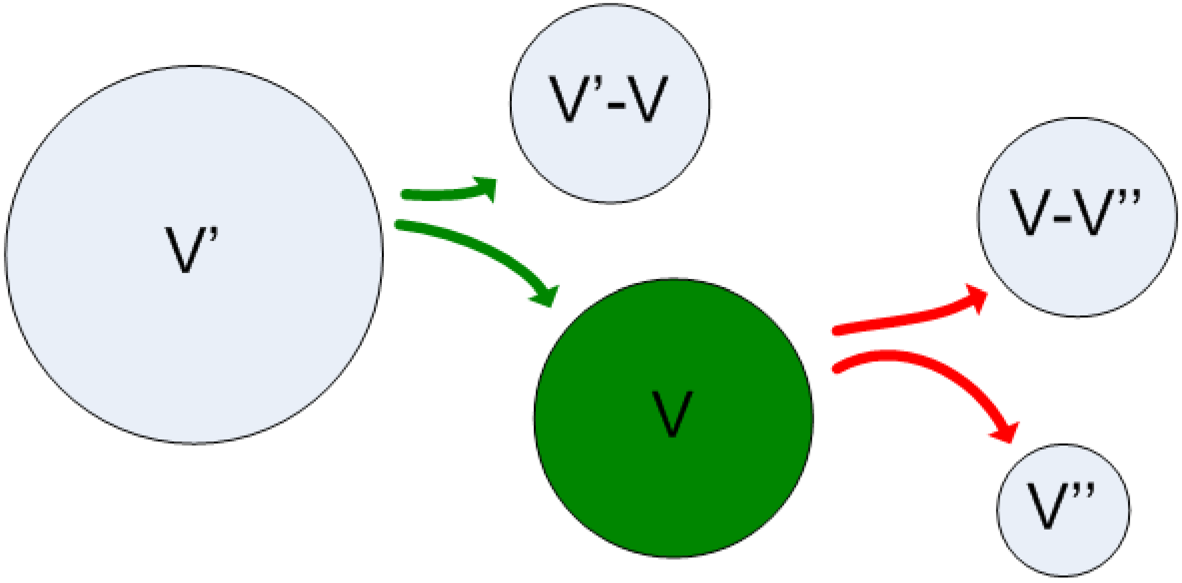
efficiency collision probability

$$\beta(V,V') = h(V,V')\ \lambda(V,V')$$

Droplet Breakup

$$S(V) = \int_V^\infty a(V')\ b(V|V')\ f_0(V')\ dV'$$

$$-\ a(V)\ f_0(V)$$

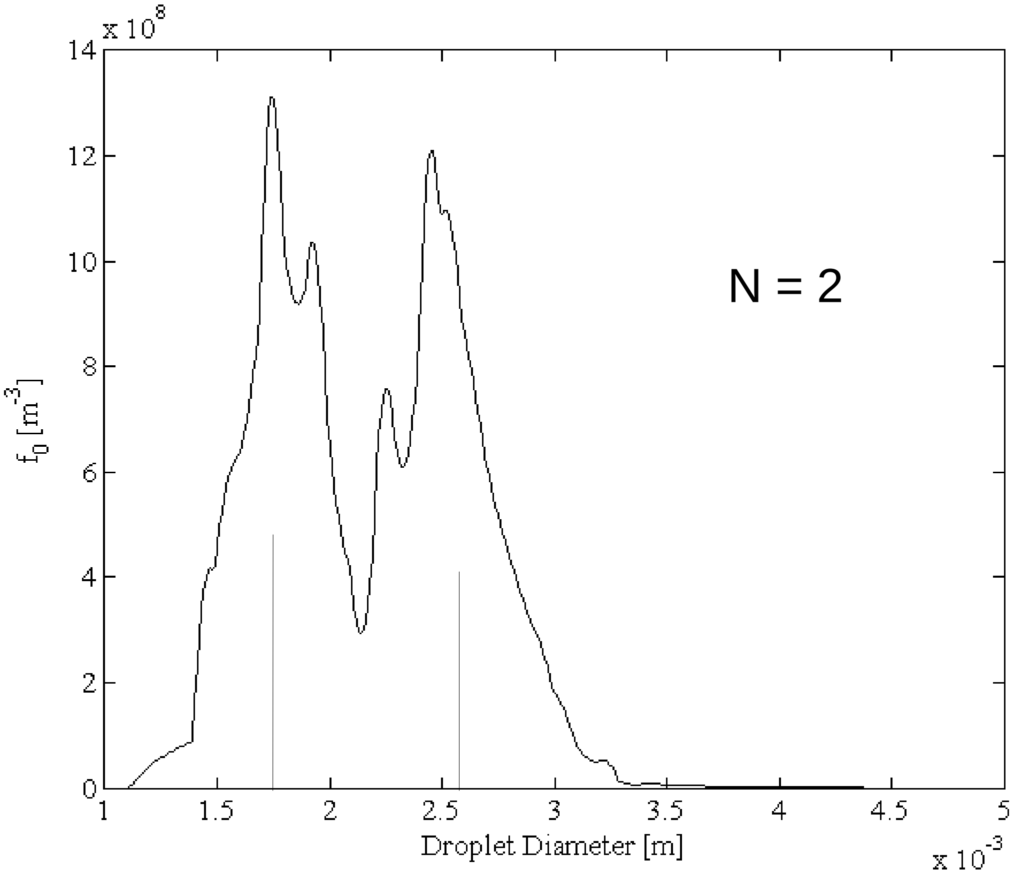


Numerical Methods

Quadrature Approximation

$$m_k = \int_0^\infty L^k \, f_0(L) \, \mathrm{d}L$$

$$\approx \sum_{i=0}^{N} w_i L_i^k$$



Solving the PBE - QMoM

QMoM

- Transport moments
- To evaluate the source terms, the quadrature weights and positions must be calculated from the moments.

$$\frac{\partial m_k}{\partial t} + \nabla \cdot (\boldsymbol{u}_d m_k) = S_k$$

$$\begin{aligned} S_k = & \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} a(L_i, L_j)\ w_i w_j \left(L_i^3 + L_j^3\right)^{k/3} \\ & - \sum_{i=1}^{N} \sum_{j=1}^{N}\ a(L_i, L_j)\ w_i w_j L_i^k \\ & + \sum_{i=1}^{N} w_i \int_0^{\infty} L^k\ g(L_i) \beta(L, L_i) \mathrm{d}L \\ & - \sum_{i=1}^{N} w_i L_i^k g(L_i) \end{aligned}$$

Solving the PBE - DQMoM

DQMoM

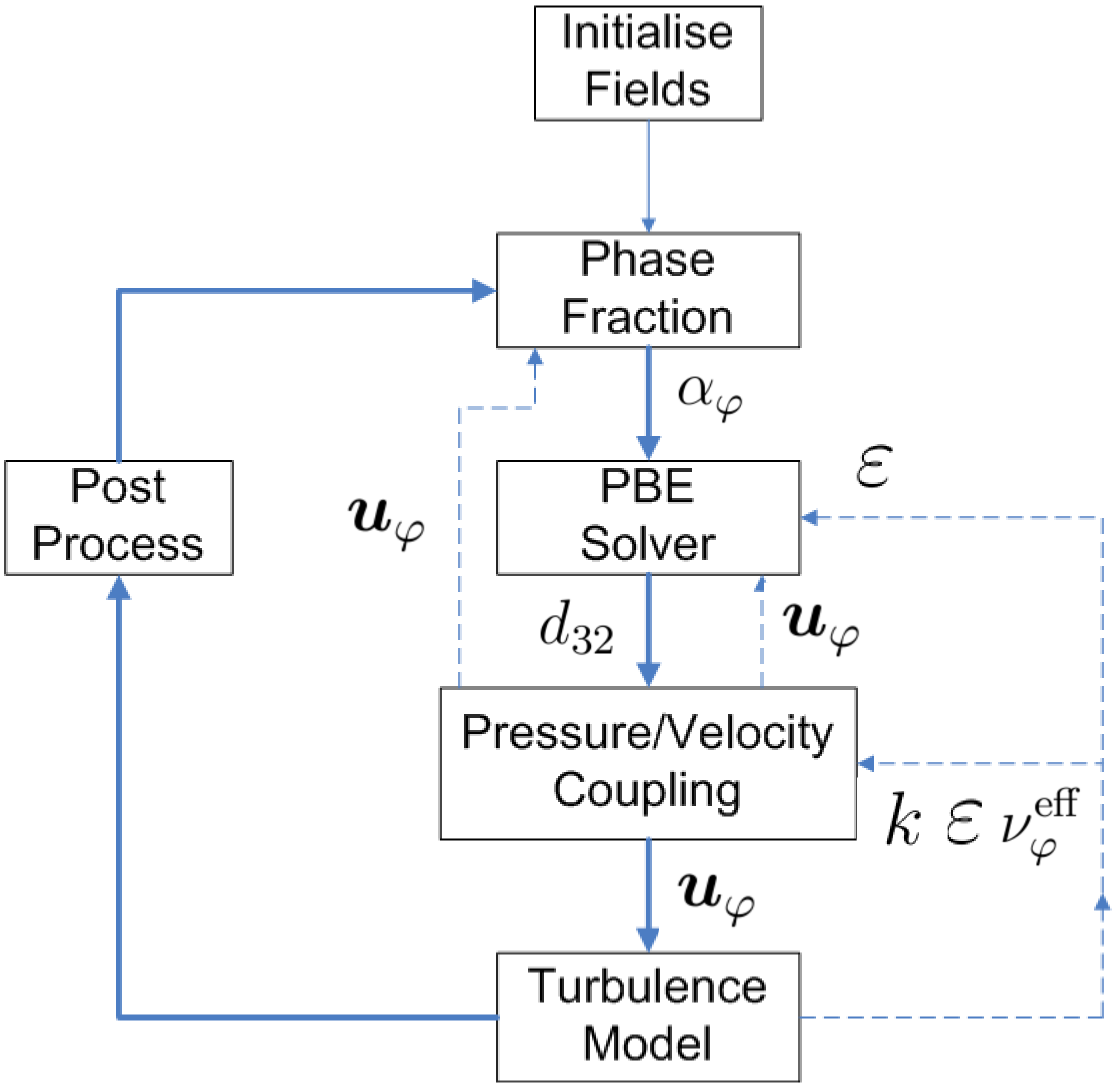
- Transport quadrature weights and weighted positions directly.
- Source terms and moments are calculated directly from these quantities.

$$\frac{\partial w_i}{\partial t} + \nabla \cdot (\boldsymbol{u}_{di} w_i) = a_i$$

$$\frac{\partial w_i L_i}{\partial t} + \nabla \cdot (\boldsymbol{u}_{di} w_i L_i) = b_i$$

$$(1-k)\sum_{i=1}^{N} L_i^k a_i + k \sum_{i=1}^{N} L_i^{k-1} b_i = S_k$$

Numerical Algorithm

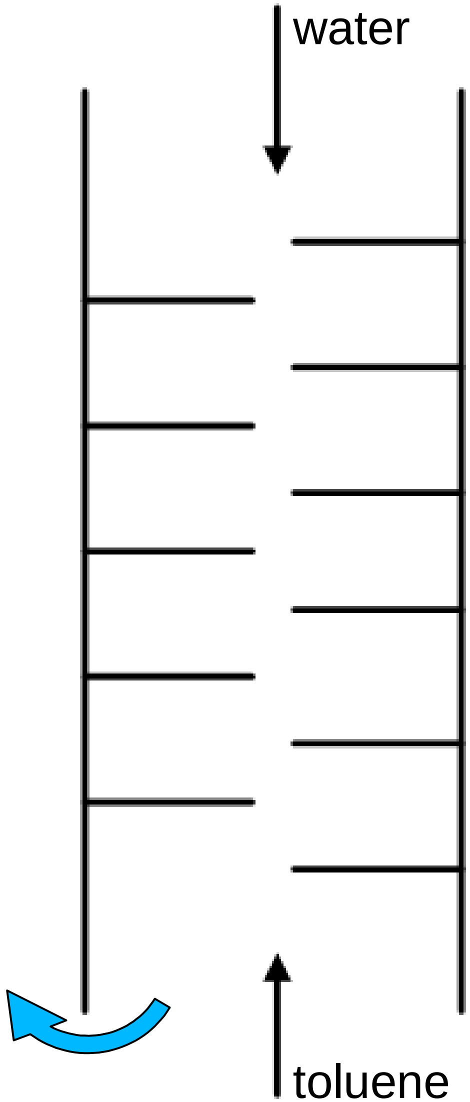


Results

Rotating disc contactor

100 L/hour of each phase.

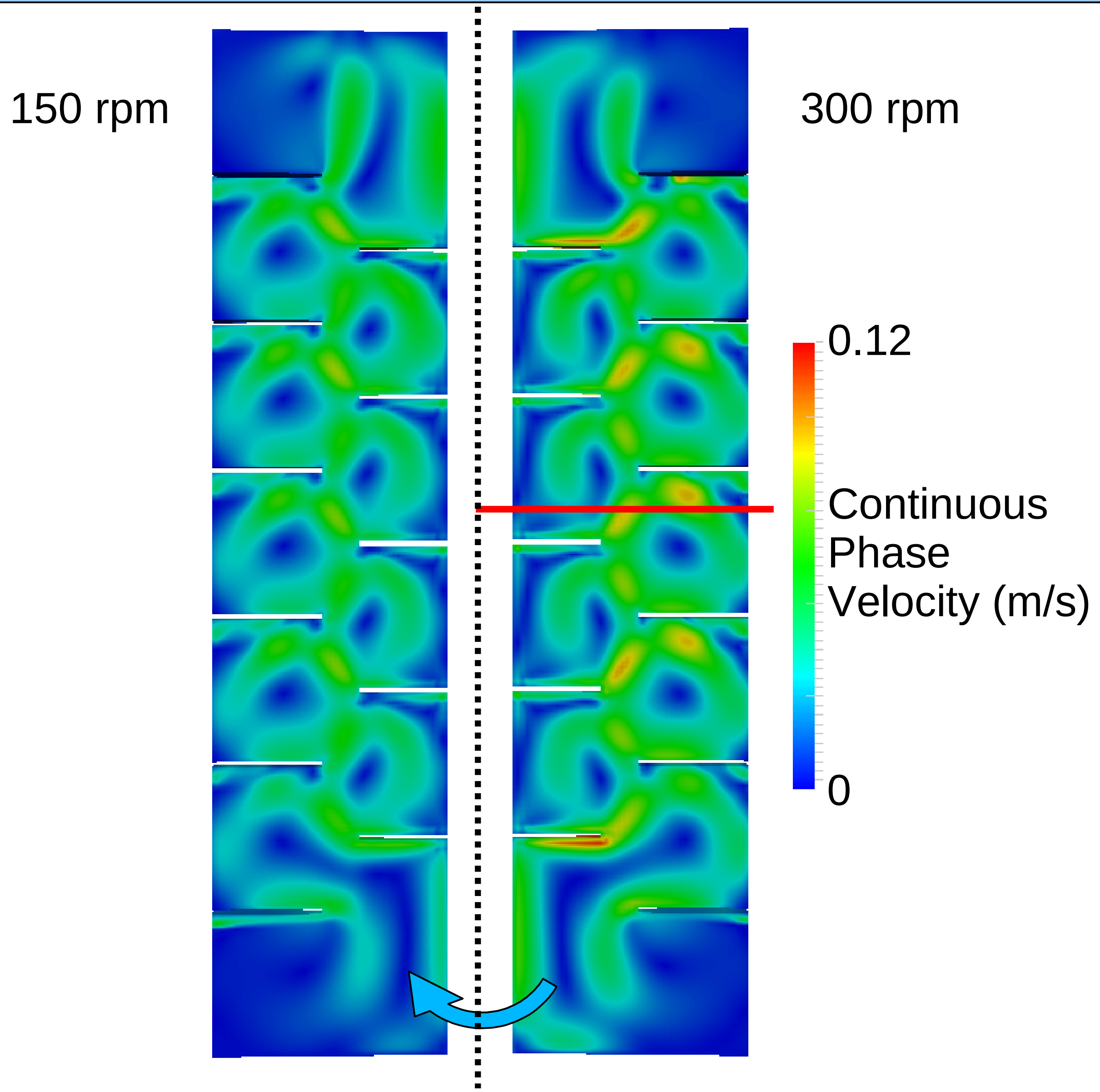
Initial volume fraction of 0.1 for toluene.



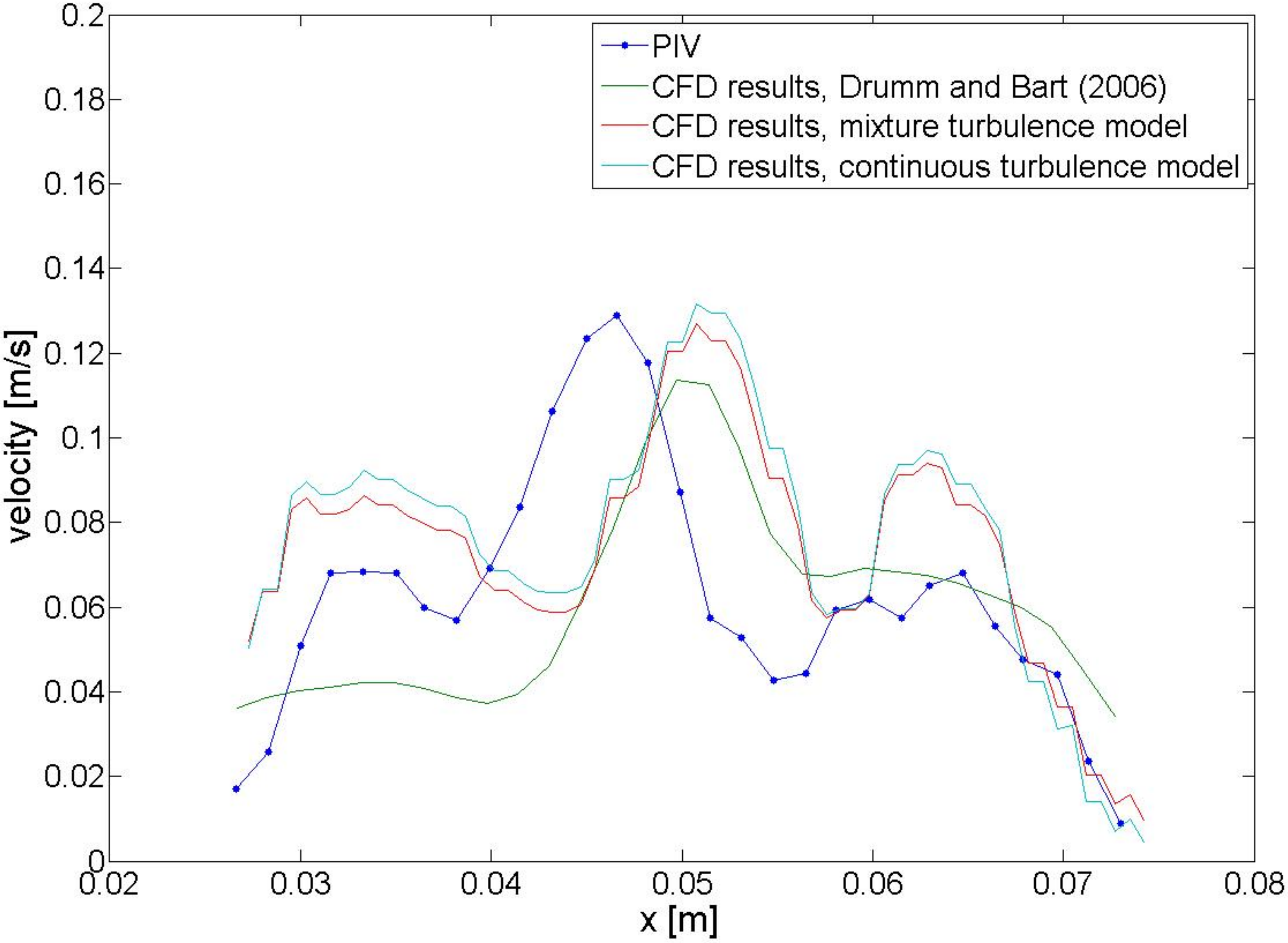
The wall’s rotation speed is changed to see the effect on the size distribution of the toluene droplets.

Rotations of 150/300 rpm are used.

RDC – continuous phase velocity

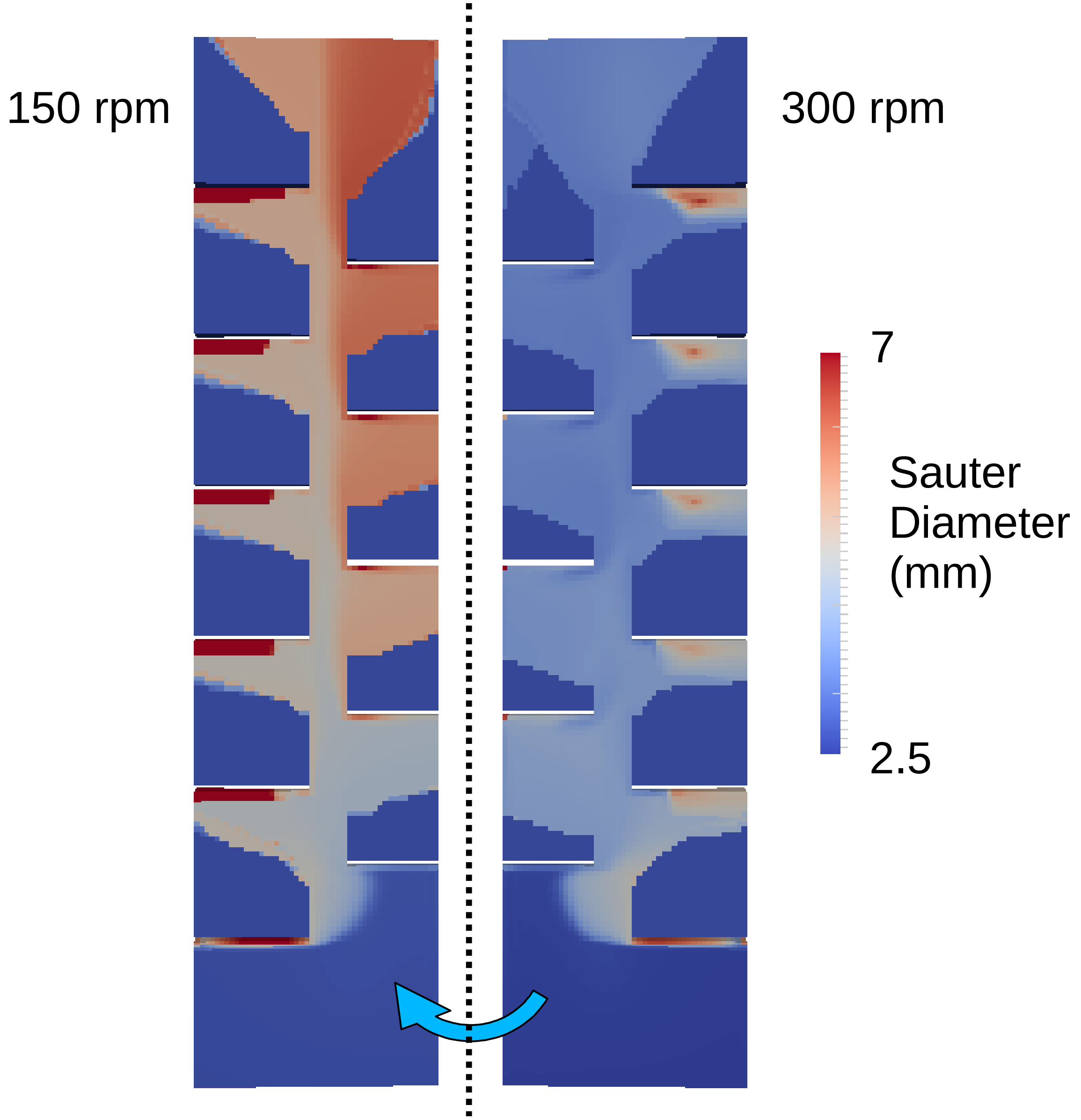


RDC – CFD only



PIV
CFD results, Drumm and Bart (2006)
CFD results, mixture turbulence model
CFD results, continuous turbulence model
velocity [m/s]
x [m]
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0.02
0.03
0.04
0.05
0.06
0.07
0.08

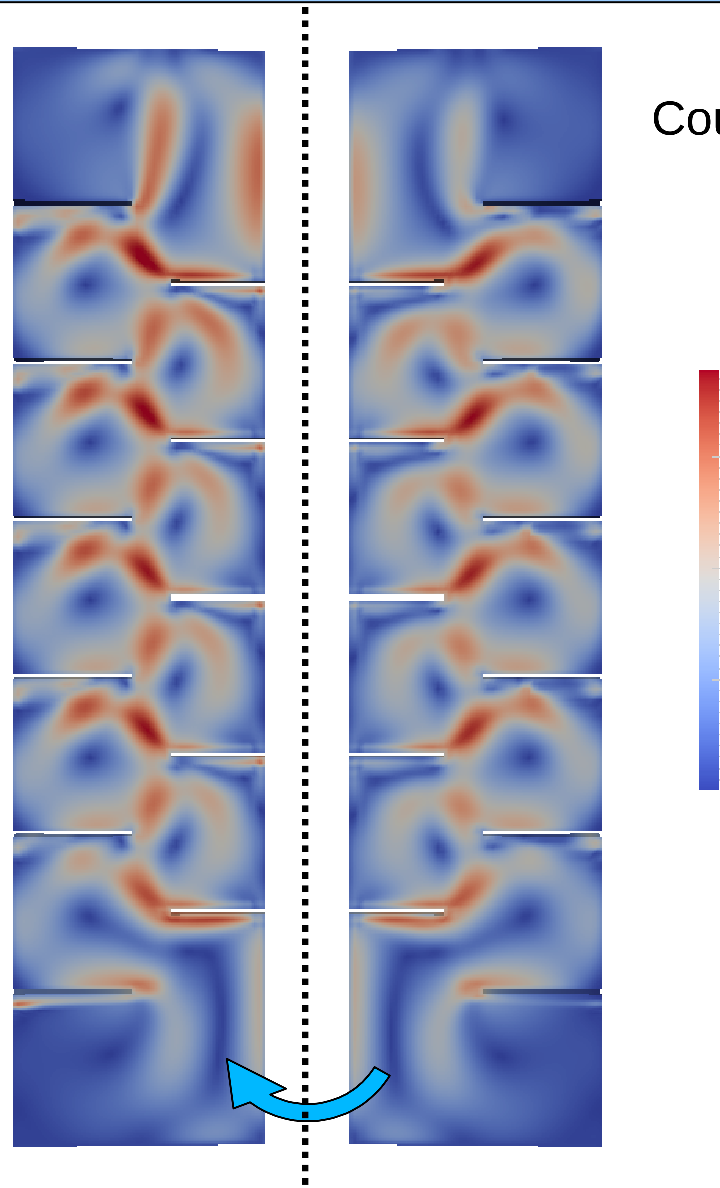
RDC – Sauter diameter



RDC – result of coupling CFD/PBE

No coupling

Coupling



Continuous Phase Velocity (m/s)

Rotation speed
150 rpm

Summary

Two moment methods have been tested and validated to solve the population balance.

A multi-fluid CFD solver has been tested and validated on a rotating disc contactor.

The PBE and CFD solvers have been coupled. The importance of that coupling has been demonstrated.

Acknowledgements

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