Predicting Size Distribution of Dispersed Phase Systems

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Outline

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- **Theory**
  - **Coupling PBE-CFD**
    - **Diffusive Transport**
  - **Modeling of Coalescence Phenomena**
  - **Modeling of Breakage Phenomena**
  - **Discretization of internal (size) coordinate**
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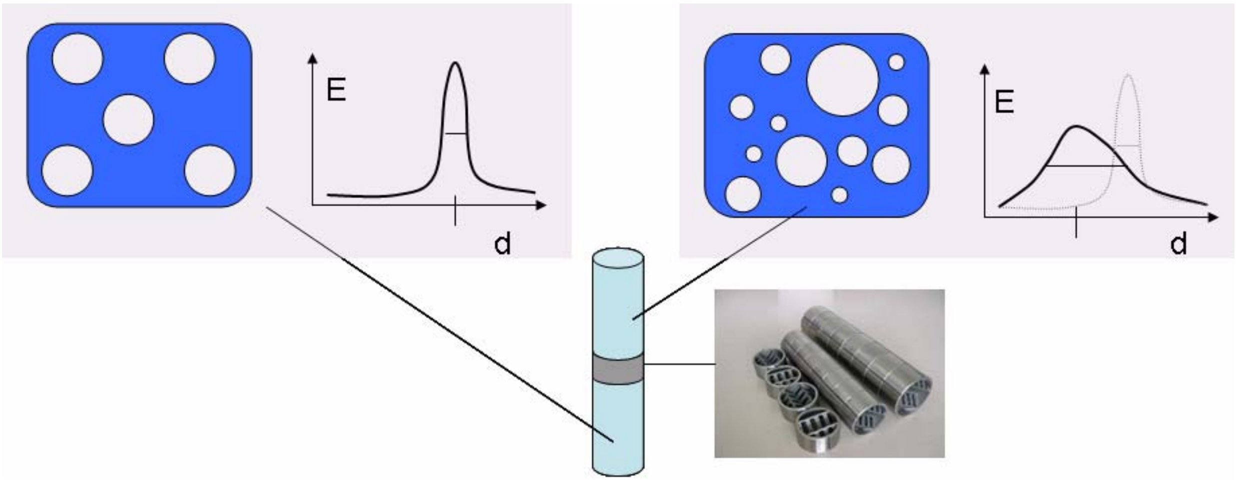
  - **High Quality CFD Data**
- **Future Plans**

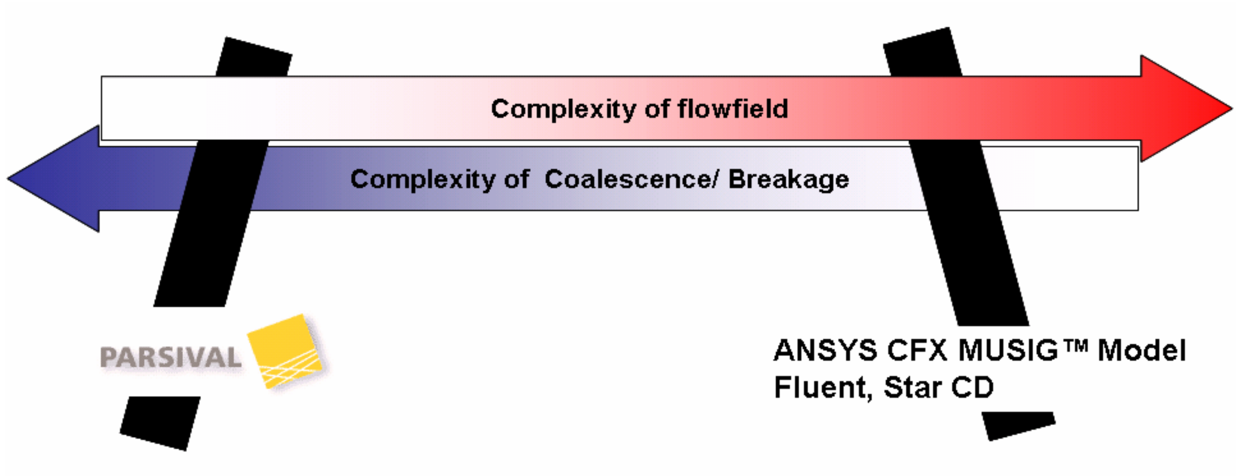
Introduction



Evolution of the size distribution of the secondary phase

- IN
  - Time
  - Spatial coordinate
  - Internal coordinate
- WITH
  - Hydrodynamic quantities
  - Physical qualities

Introduction



The effort results in an inevitable coupling of CFD and PBE.

- **No** analytical solution for practical problems!
- **No** commercial code sufficiently good for every case!
- Accurate CFD calculations for complex geometries!
- High computational costs!
- Lack of unified framework of “breakage kernel”!
- Robust, fast and accurate prediction of mixing properties!

Theory: $\mathcal{C}$-$\mathcal{D}$ Problem

$$\frac{\partial f}{\partial t} + \mathbf{u}_g \cdot \nabla f = B^+ + B^- + C^+ + C^-$$

$$\frac{\partial f}{\partial t} + \mathbf{u}_g \cdot \nabla f - \nabla \cdot (\frac{\nu_T}{\sigma_T} \nabla f) = B^+ + B^- + C^+ + C^-$$

- A scalar non-linear time dependent non-homogenous convection-diffusion problem.
- Non-homogeneity: Source and Sink terms due to
  - Coalescence
  - Breakage
- Robustness and fastness depends on the numerical schemes.
- Accuracy depends on modeling of source and sink terms.

Theory: PBEs

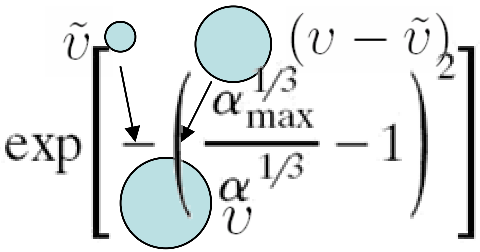
$$\frac{\partial f}{\partial t} + \mathbf{u}_g \cdot \nabla f = \int_v^\infty r^B(v,\tilde{v}) f(\tilde{v})\, d\tilde{v} - \frac{f(v)}{v} \int_0^v \tilde{v} r^B(\tilde{v}, v)\, d\tilde{v}$$
$$+ \frac{1}{2} \int_0^v r^C(\tilde{v}, v - \tilde{v}) f(\tilde{v}) f(v - \tilde{v})\, d\tilde{v} - f(v) \int_0^\infty r^C(\tilde{v}, v) f(\tilde{v})\, d\tilde{v},$$

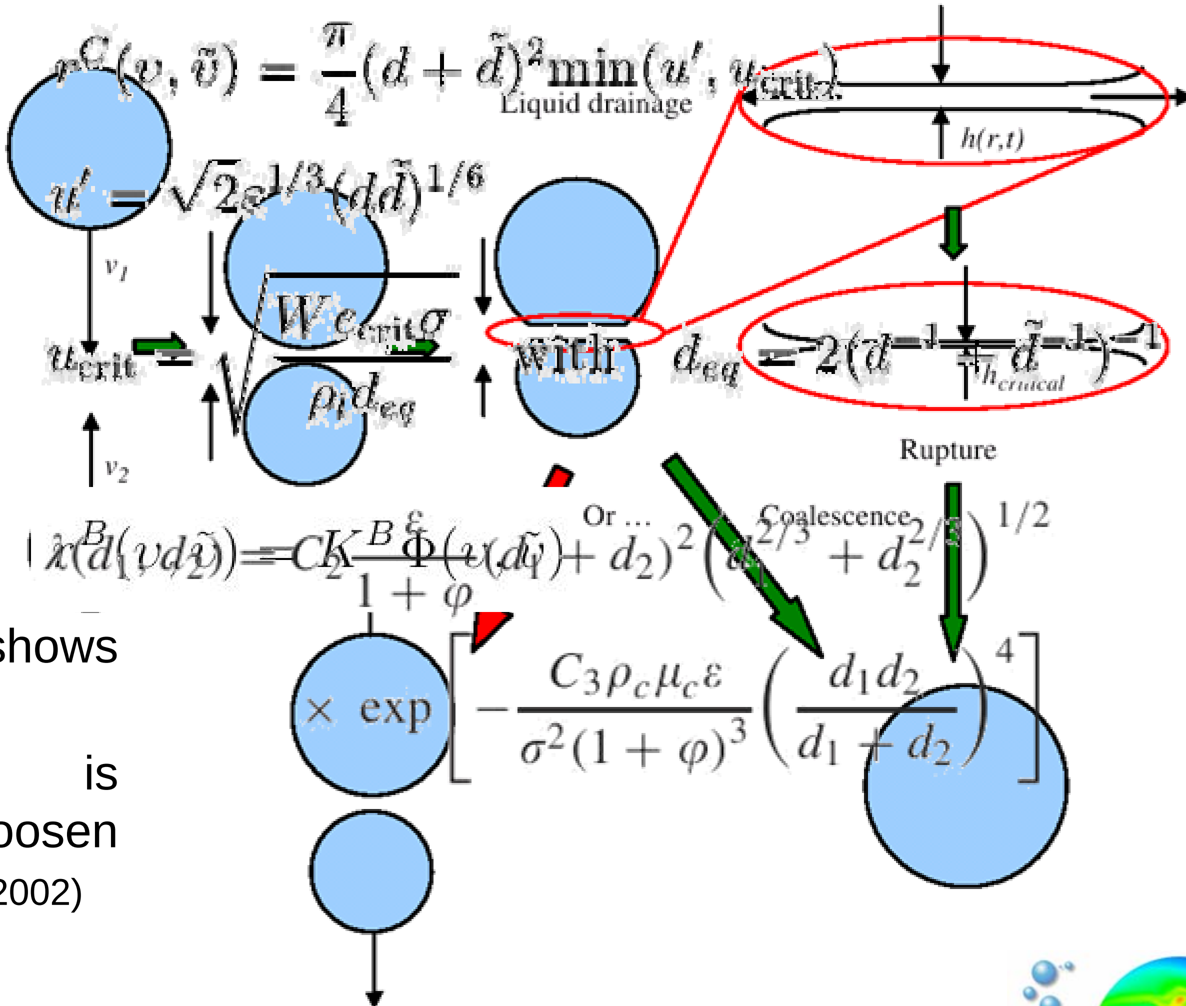
PBEs are introduced into $\mathcal{C}$-$\mathcal{D}$ problem

- An integro-differential equation
  - which has to be treated very carefully!
  - which has to be closed with proper kernels to obtain **accurate** results.
  - which has to be discretized with proper techniques to obtain **robust** and **fast** solvers.

Theory: Kernels

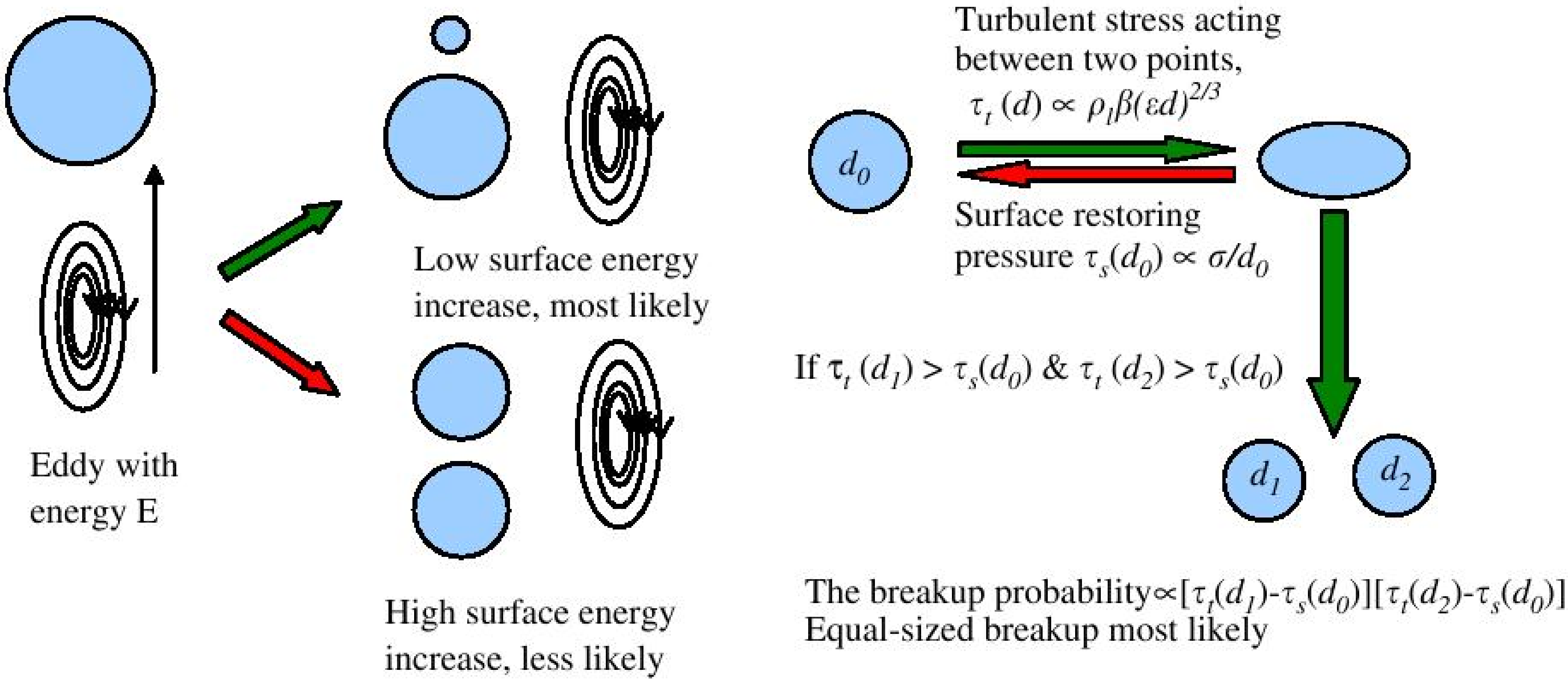
- Coalescence kernel





- Breakage kernel
- Most of the models shows the similar trends.
- Equlibrium BSD is independent of choosen model. (Buwa&Ranade, 2002)

Theory: Breakage kernel



(a) Luo and Svendsen

(b) Martínez-Bazán et al.

Theory: Breakage kernels

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Lee et						
Hesket Hesket	√	√	X	√	√	√
Nambi						
Tsouri	√	√	√	X	√	√
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Martin	√	√	√	√	√	X
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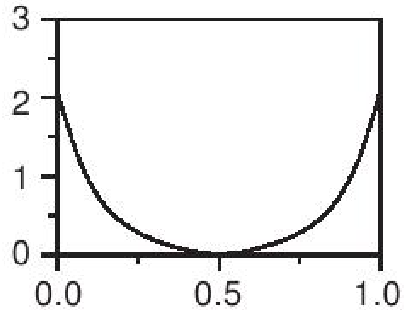
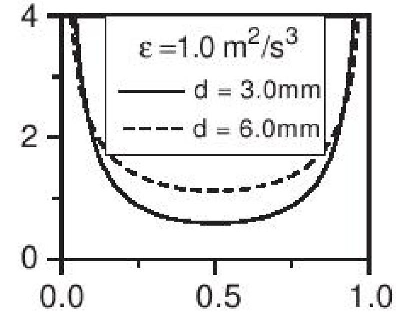
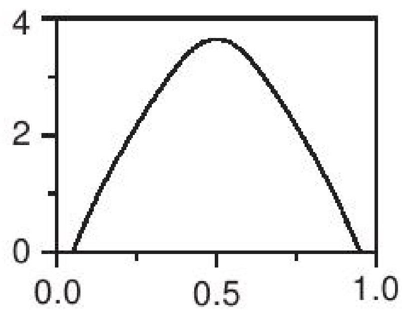
Lehr a						



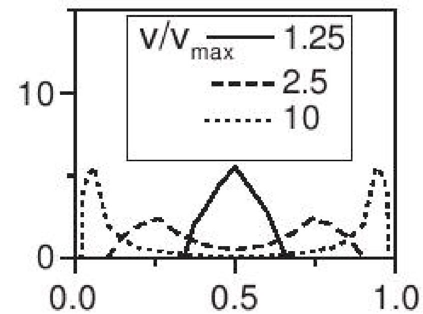
Tsouris and Tavlarides (1994)



Luo and Svendsen (1996)



Martínez-Bazán et al. (1999)



Lehr and Mewes (2001)

Hesketh and Etchells (1991a), Hesketh et al. (1991b)

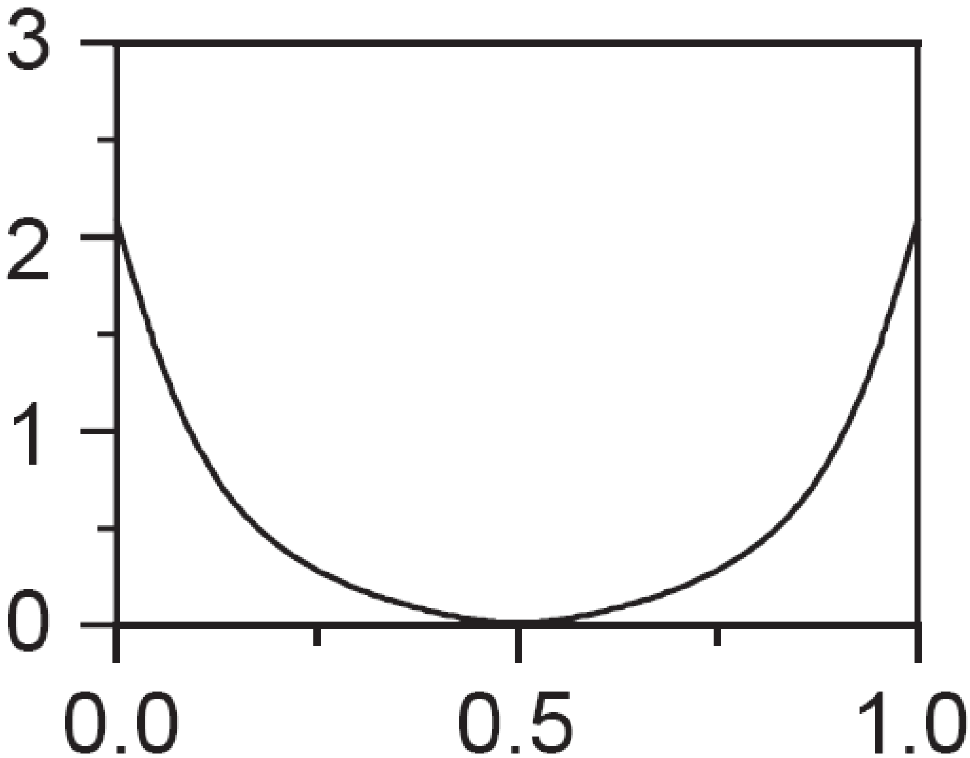
Nambiar et al. (1992)

Theory: Tsouris & Tavlarides

$$g(d) = k_8 D F(\phi) \epsilon_i^{1/3} \int_{2/d}^{2/de,min} (2/k + d)^2 (8.2k^{-2/3} + 1.07d^{2/3})^{1/2} exp(-E_c/C_1 e) dk n_d$$

- Geometric parameter k_8: ratio of impeller volume to tank volume.
- Empirical parameter C_1: found by LSF to measured data.
- The breakage frequency is **too much** problem specific!

Theory: Tsouris & Tavlarides



- ϵ_{min} : en   e.
- ϵ_{max} : en
- ϵ_{d} : su
- **Unequal**

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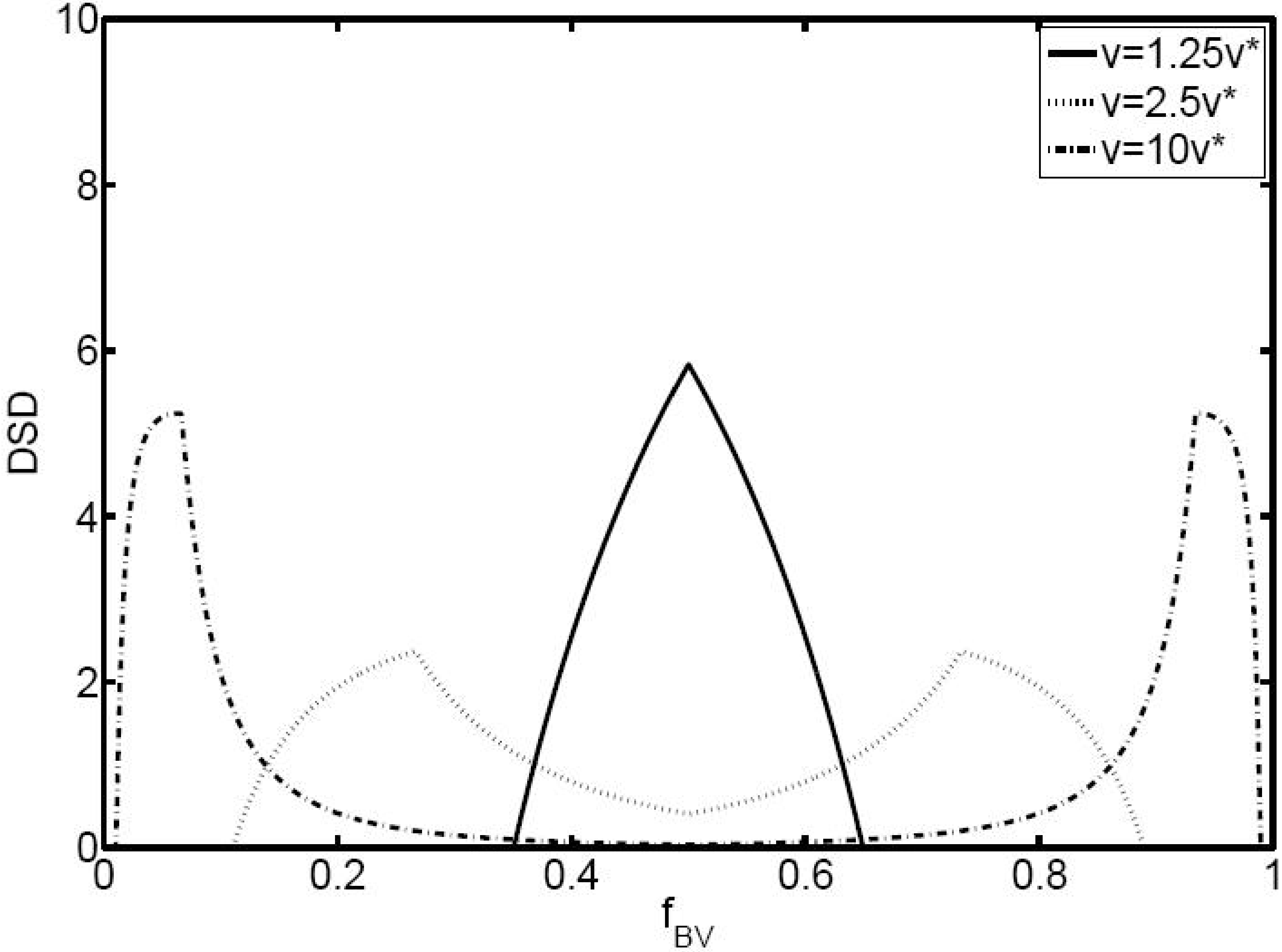
K

$\Phi($



Theory: Lehr et al., 2002

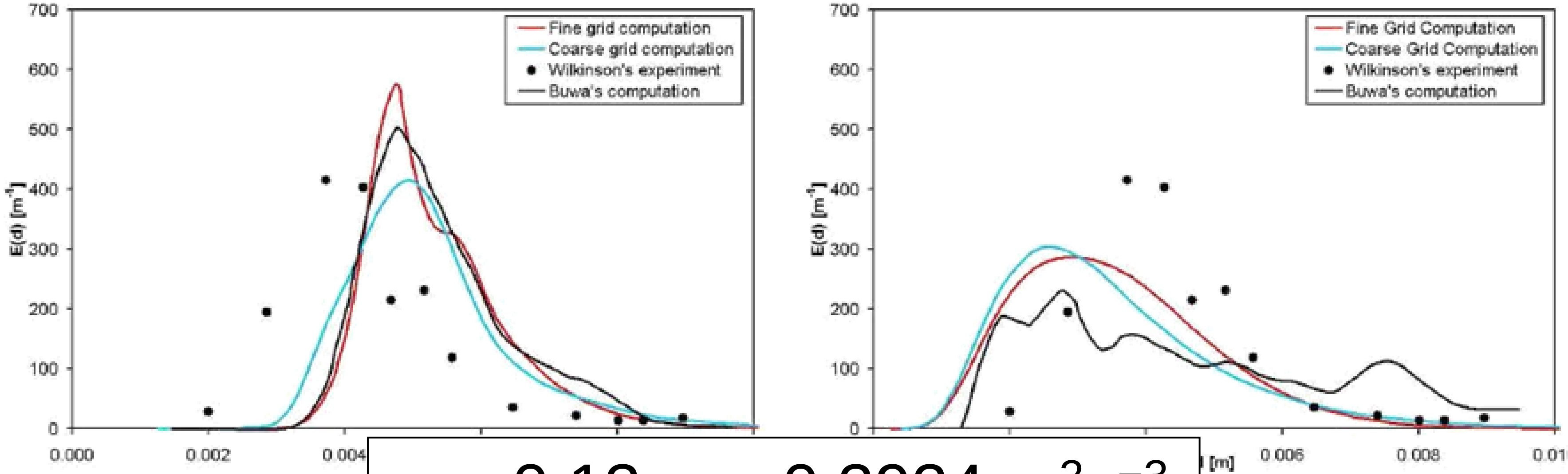
$$K^B = \frac{{d^*}^{5/3}}{2T} \exp\left(-\frac{\sqrt{2}}{{d^*}^3} \right)$$

$$\phi(\upsilon, \tilde{\upsilon}) = \frac{6}{\left(L\sqrt{\pi}\tilde{d}^* \right)^3} \frac{\exp\left(-2.25 \left(\ln\left(2^{2/5}\tilde{d}^* \right) \right)^2 \right)}{1 + \operatorname{erf}\left(\ln\left(2^{1/15} d^* \right)^{1.5} \right)}$$

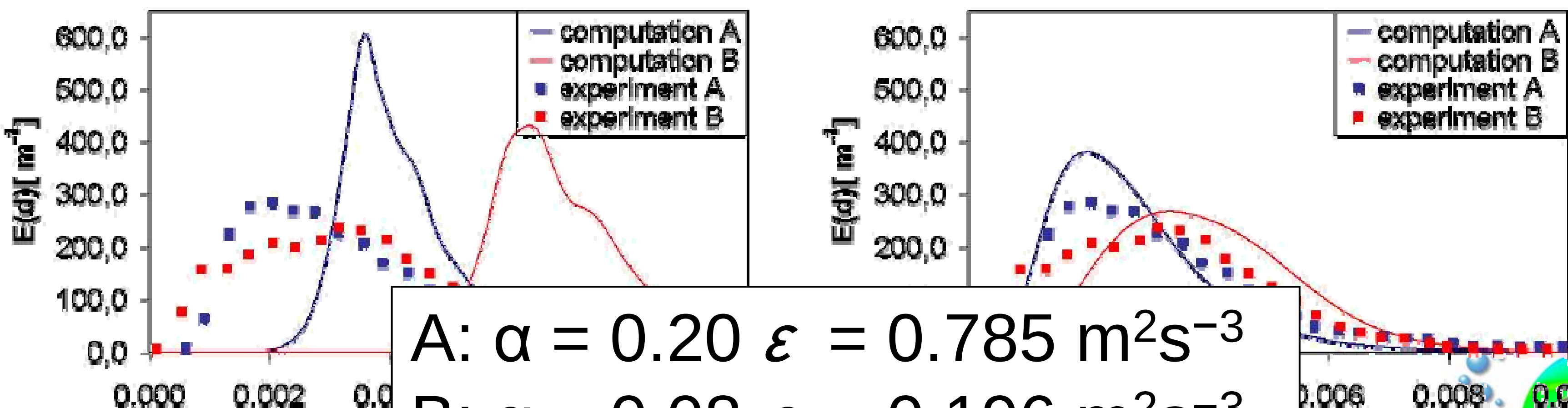
- Work with non-dimesional parameters for wide range of operating conditions.
- Charecteristic time, length are introduced.

$$T = \left(\frac{\sigma}{\rho_L} \right)^{0.6} \frac{1}{\varepsilon^{0.4}} \qquad L = \left(\frac{\sigma}{\rho_L} \right)^{0.4} \frac{1}{\varepsilon^{0.6}}$$

Theory: Lehr et al., 2002



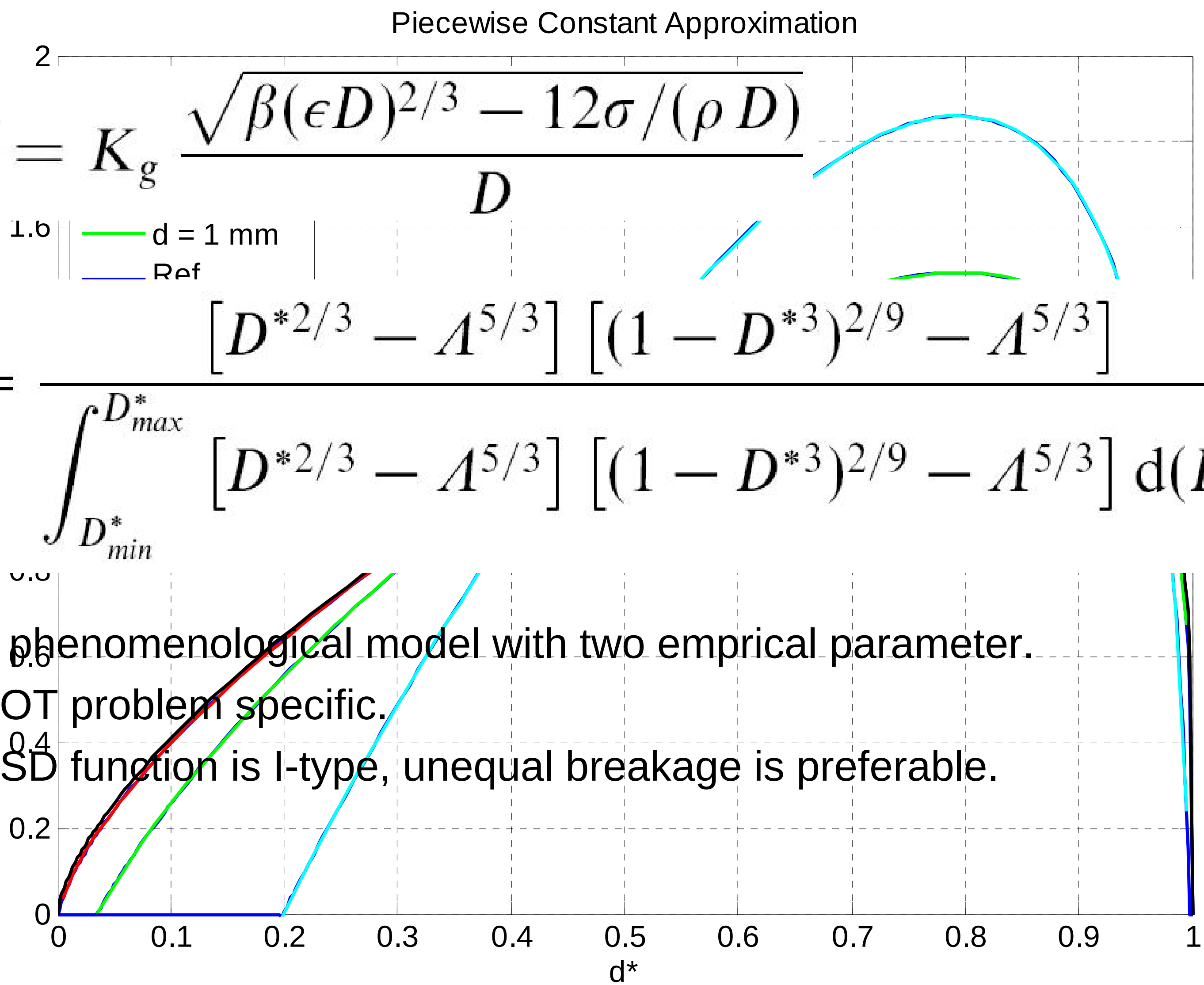
$\alpha = 0.13$ $\varepsilon = 0.3924\ m^2s^{-3}$



A: $\alpha = 0.20$ $\varepsilon = 0.785\ m^2s^{-3}$

B: $\alpha = 0.08$ $\varepsilon = 0.196\ m^2s^{-3}$

Theory: Martinez et al., 1999



$$K^B = K_g \frac{\sqrt{\beta(\epsilon D)^{2/3} - 12\sigma/(\rho D)}}{D}$$

$$\Phi = \frac{\left[D^{*2/3} - \Lambda^{5/3}\right]\left[(1 - D^{*3})^{2/9} - \Lambda^{5/3}\right]}{\int_{D^*_{min}}^{D^*_{max}} \left[D^{*2/3} - \Lambda^{5/3}\right]\left[(1 - D^{*3})^{2/9} - \Lambda^{5/3}\right] \mathrm{d}(D^*)}$$

- A phenomenological model with two emprical parameter.
- NOT problem specific.
- DSD function is I-type, unequal breakage is preferable.

Theory: Size Discretization

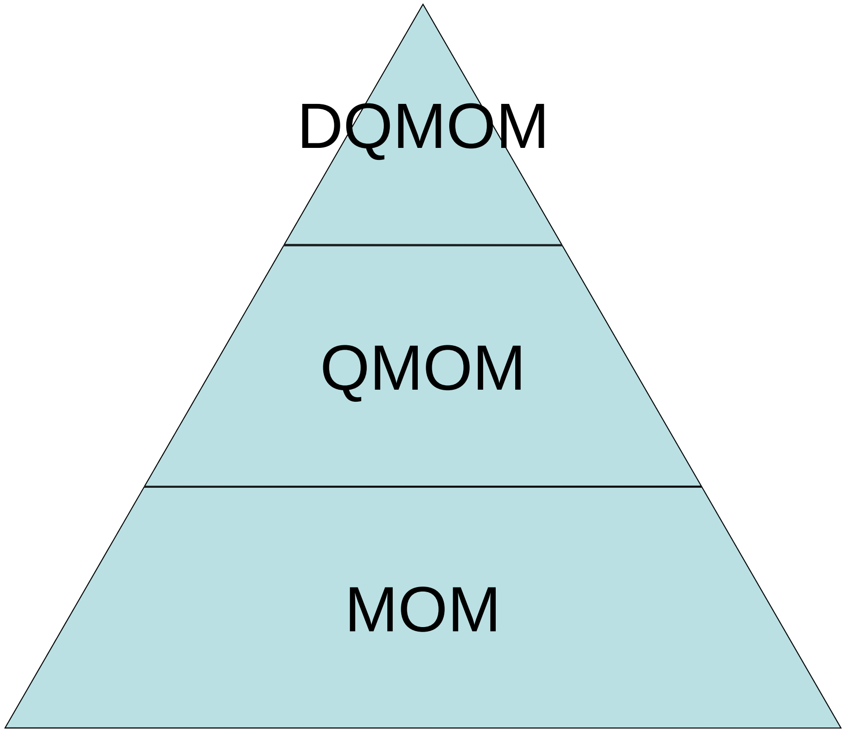
To solve the integro-differential PBE for practical applications, the integrals should be discretized with a proper discretization technique.

- Method of Moments (MOM), *McGraw and Saunders, 1984*
- Quadrature Method of Moments (QMOM), *Marchsio et al., 2003*
- Direct Quadrature Method of Moments (DQMOM), *Marchsio et al., 2005*
- Parallel Parent Daughter Classes (PPDC), *Bove et al., 2005*
- Method of Classes (MC), *Kumar and Ramkrishna, 1996*
- Cell Averaged Technique (CAT), *Kostoglou, 2007*

IF THE DISCRETIZATION IS FINE ENOUGH, THE RESULT SHOULD BE INDEPENDENT OF THE CHOSEN METHOD! ?

Theory: D/Q/MOM

- All is based on formulating a tracer equation for moments or abscissas and weights.
- MOM: the key is to formulate the problem in terms of the moments in closed forms.
- MOM can be used when the source and sink terms directly computed. Which is possible only for growth terms.
- MOM is extended to QMOM for breakage and coalescence.
- DQMOM avoids the PD algorithm which is used in QMOM and tracks the abscissas and weights.



Theory: D/Q/MOM

Reformulation of the problem in terms of moments

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

$$\overline{D_k^a}(\mathbf{x},t) = \int_0^{+\infty} L^k n(L;\mathbf{x},t)\int_0^{+\infty}\beta(L,\lambda) \times n(\lambda;\mathbf{x},t)\,\mathrm{d}\lambda\,\mathrm{d}L,$$

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

$$\overline{D_k^b}(\mathbf{x},t) = \int_0^{+\infty} L^k a(L)n(L;\mathbf{x},t)\,\mathrm{d}L$$

$$\frac{\partial m_k(\mathbf{x},t)}{\partial t} + \langle u_i\rangle \frac{\partial m_k(\mathbf{x},t)}{\partial x_i} - \frac{\partial}{\partial x_i}\left[\Gamma_t \frac{\partial m_k(\mathbf{x},t)}{\partial x_i}\right]$$

$$= \frac{1}{2} \sum_i w_i \sum_j w_j (L_i^3 + L_j^3)^{k/3} \beta_{ij} - \sum_i L_i^k w_i \sum_j \beta_{ij} w_j$$

$$+ \sum_i a_i \bar{b}_i^{(k)} w_i - \sum_i L_i^k a_i w_i$$

where $\beta_{ij} = \beta(L_i, L_j)$, $a_i = a(L_i)$, and

$$\bar{b}_i^{(k)} = \int_0^{+\infty} L^k b(L|L_i)\,\mathrm{d}L.$$

$i = 1$

MC formulation of the problem yields,

$$\frac{\partial f_i}{\partial t} + \mathbf{u}_g \cdot \nabla f_i = \sum_{j=i}^{n} r^B_{i,j} f_j \Delta v_j - \frac{f_i}{v_i} \sum_{j=1}^{i} v_j r^B_{j,i} \Delta v_j$$

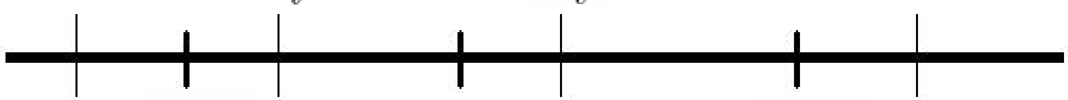
$$v_i - \frac{2}{3}(v_i - v_{i-1})$$

$$\ldots 2 \sum_{j=1} \ldots_{j,k} f_j f_k \Delta v_j \ldots \sum_{j=1} \ldots$$

$$v_i + \frac{1}{3}(v_{i+1} - v_i)$$

$$v_i^L \qquad v_i^U$$

$$\frac{\partial m_k(\mathbf{x},t)}{\partial \ldots} \ldots \mathbf{x},t) \quad \partial \quad \partial m_k(\mathbf{x},t)]$$



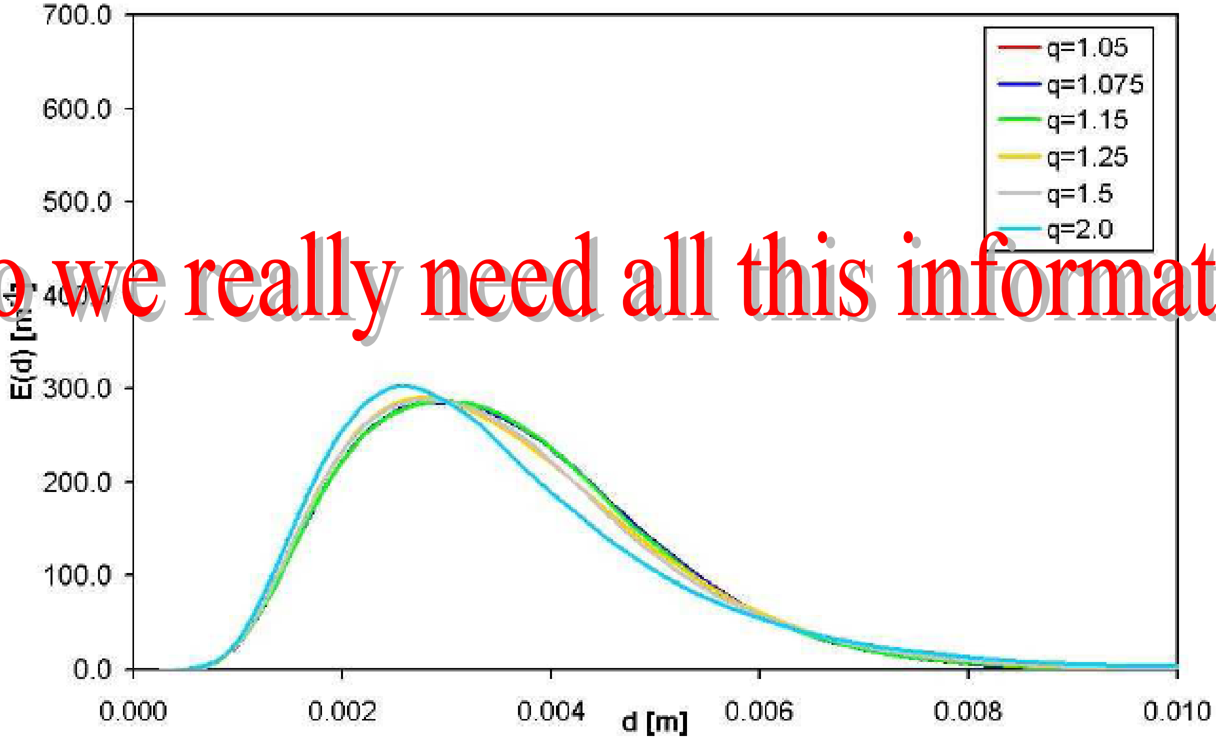
$$= \frac{1}{2} \sum_i w_i \sum_j w_j (L_i^3 + L_j \ldots)^{\ldots 3} \beta_{ij} - \sum_i L_i^k w_i \sum_j \beta_{ij} w_j$$

$$+ \sum_i a_i \bar{b}_i^{(k)} w_i - \sum \ldots$$

$$v_{\min} q^{i-1}$$

Theory: MC & PPDC

What's a good value for discretization constant *q* ?



Lehr et al., 2002

Do we really need all this information?

Theory: MC & PPDC

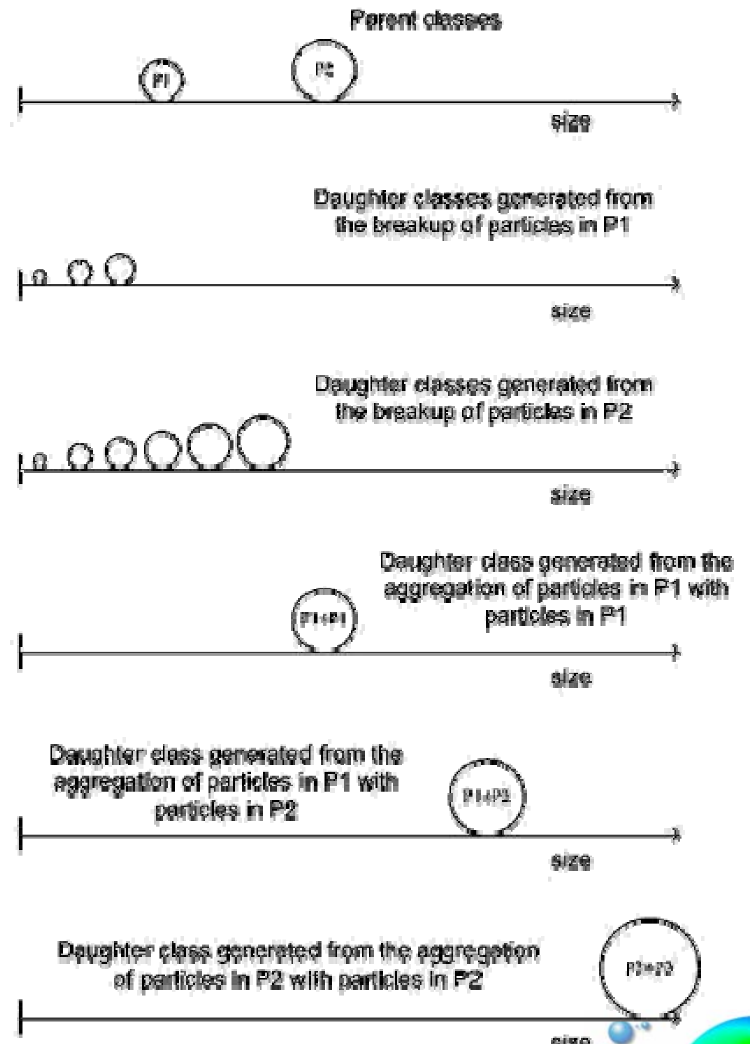
Generally, initial condition of our problems is a dirac function or superposition of few.

$$f_E(v,t) = \sum_{i=1}^{M} N_i(t)\delta(v - x_i)$$

$$f_E(v,t) = \underbrace{\sum_{i=1}^{M} N_i(t)\delta(v - x_i)}_{\text{parents-classes}}$$

$$+ \underbrace{\sum_{i=1}^{M}\sum_{j=i}^{M} A_{ij}(t)\delta(v - y_{ij})}_{\text{agglomeration-daughter-classes}}$$

$$+ \underbrace{\sum_{i=1}^{M}\sum_{k=1}^{NB(i)} B_k^{(i)}(t)\delta(v - z_k^{(i)})}_{\text{breakage-daughter-classes}}$$



Bove et al., 2005

Theory: MC & PPDC

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The key is product difference algorithm. (Gordon, 1968; Bove et al., 2005)

$$\sum_{i=1}^{M} \tilde{N}_i \tilde{x}_i^k = m_E^k(t^{n+1}), \quad k = 0, \ldots, 2M-1$$

i. BSD with M parent classes at t^n.
ii. Generating the new expanded BSD at t^{n+1}.
iii. Calculate the first 2M moments of the new expanded BSD.
iv. Obtain the reduced BSD with M classes by using PD algorithm.
v. Repeat this until $t^{n+1} \leq T_{max}$.

i. Construction of matrix ***P***.
ii. Compute the vector α with entries of ***P***.
iii. Assemble the symmetric tridiagonal matrix ***J*** with entries of α.
iv. Eigenvalues of ***J*** are the abscissas of reduced PSD and the number densities can be found by the first entries of corresponding eigenvectors.

Theory: MC & PPDC

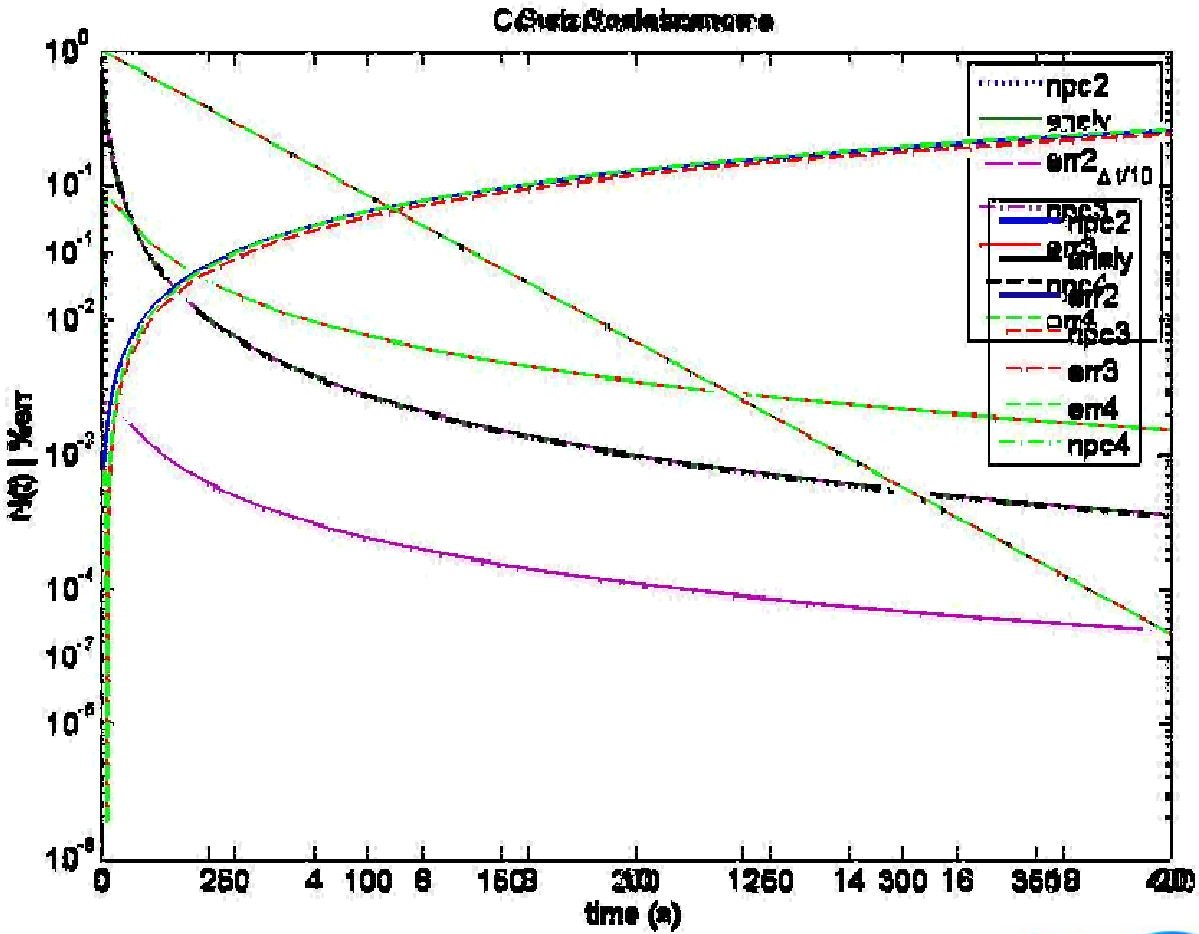
$$a(v, v') = C(v + v')$$

$$N(t) = N_0 e^{-C N_0 v_0 t}$$

$N_0 = 1,\ C = 1,\ v_0 = 1$

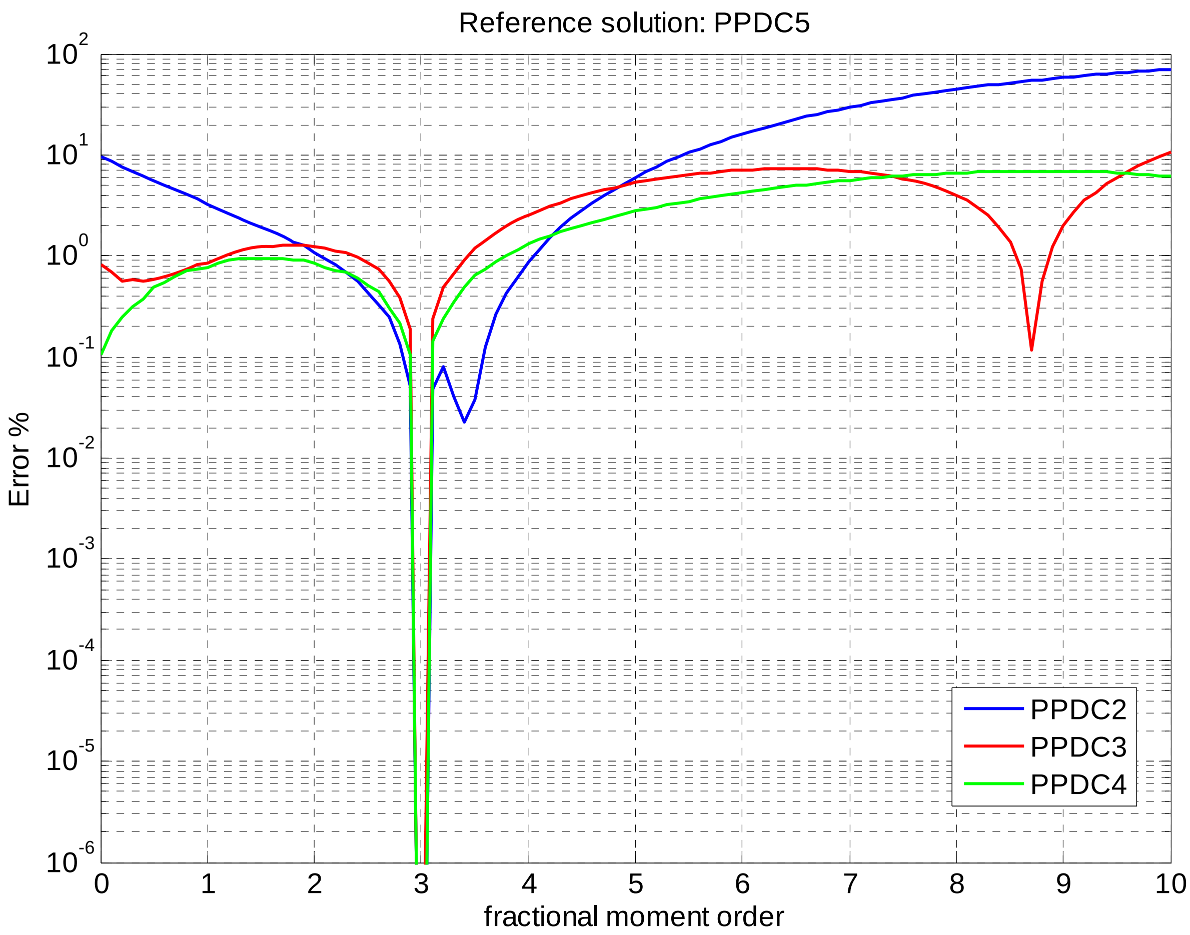
$$N(t) = \frac{2 N_0}{C N_0 t + 2}$$

$N_0 = 1\ \&\ C = 1$



Comparison of MC and PPDC for the following case:

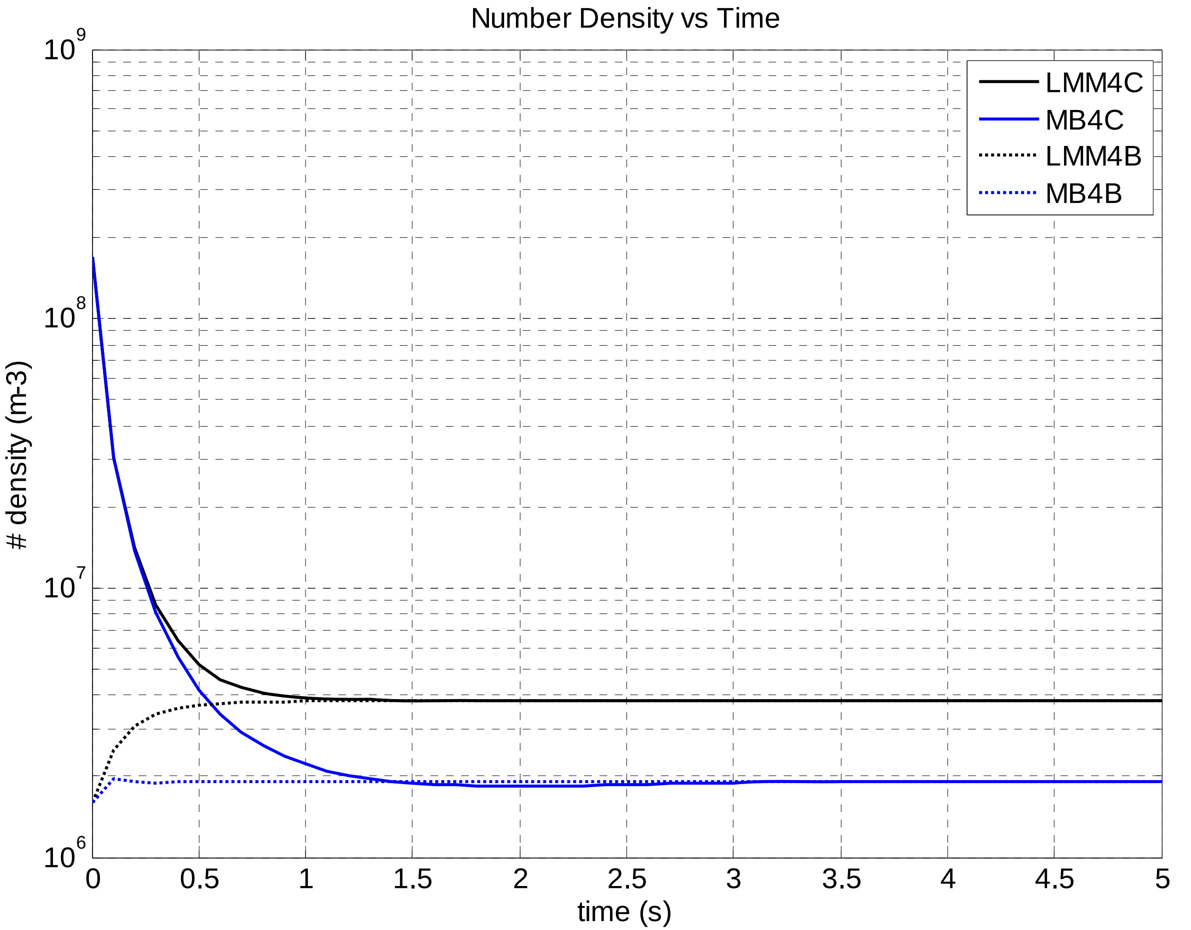
$\alpha = 0.18$, $\varepsilon = 0.3924$, water-air mixture



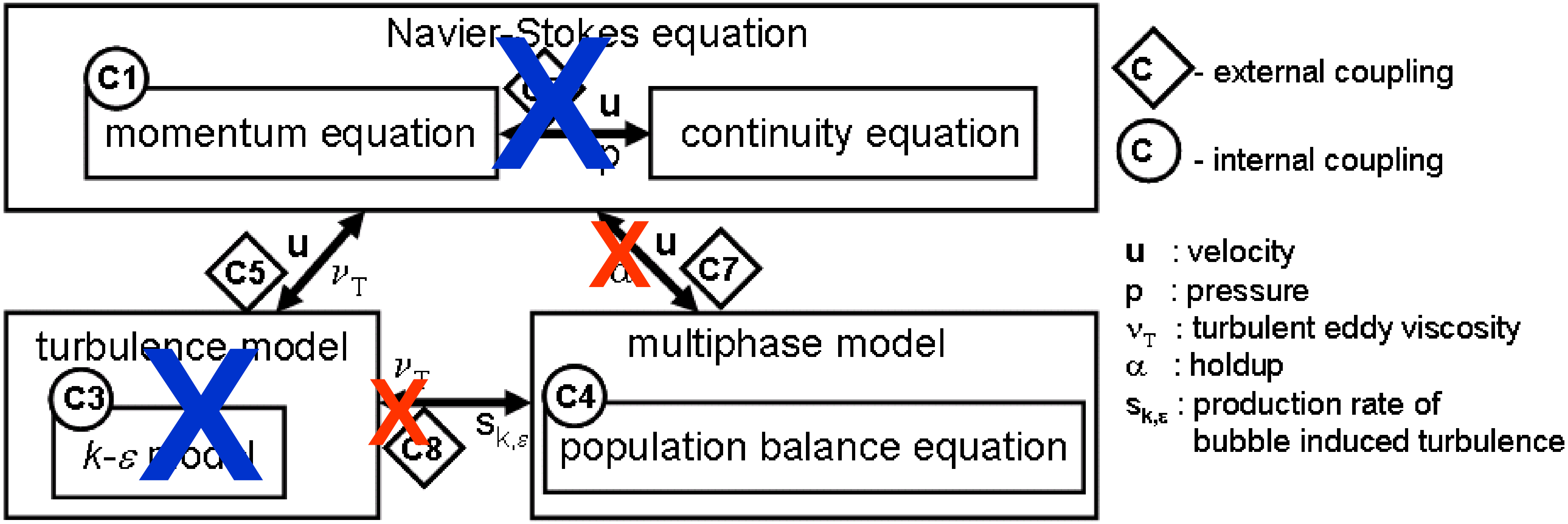
Theory: PPDC with LMM & MB

Convergence of different models with 2,3, and 4 Particle classes.

Simulation of coalescence and breakage, dominant cases.



Non-stationary two way coupled, CFD - PBE.



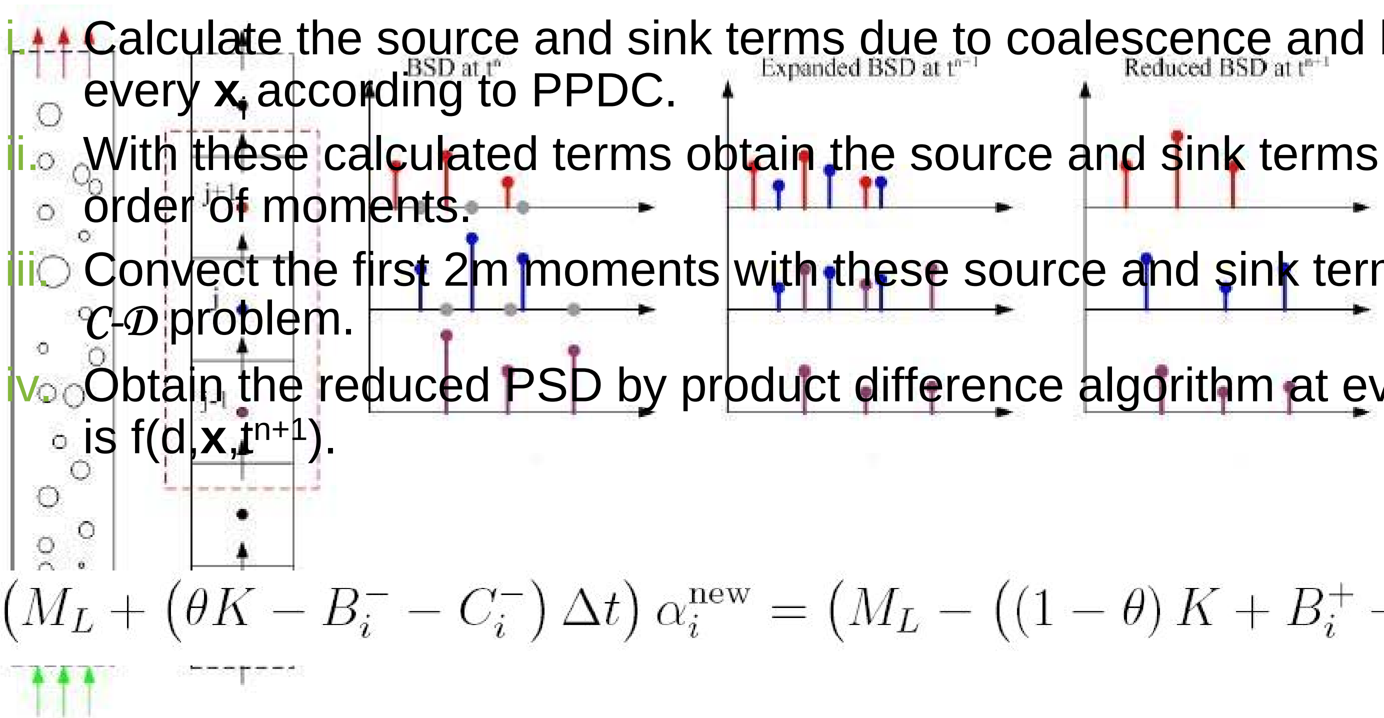
Non-stationary one way coupled, CFD - PBE. X

Stationary one way coupled, CFD - PBE. X

Suggested by Bove (Bove, 2005)

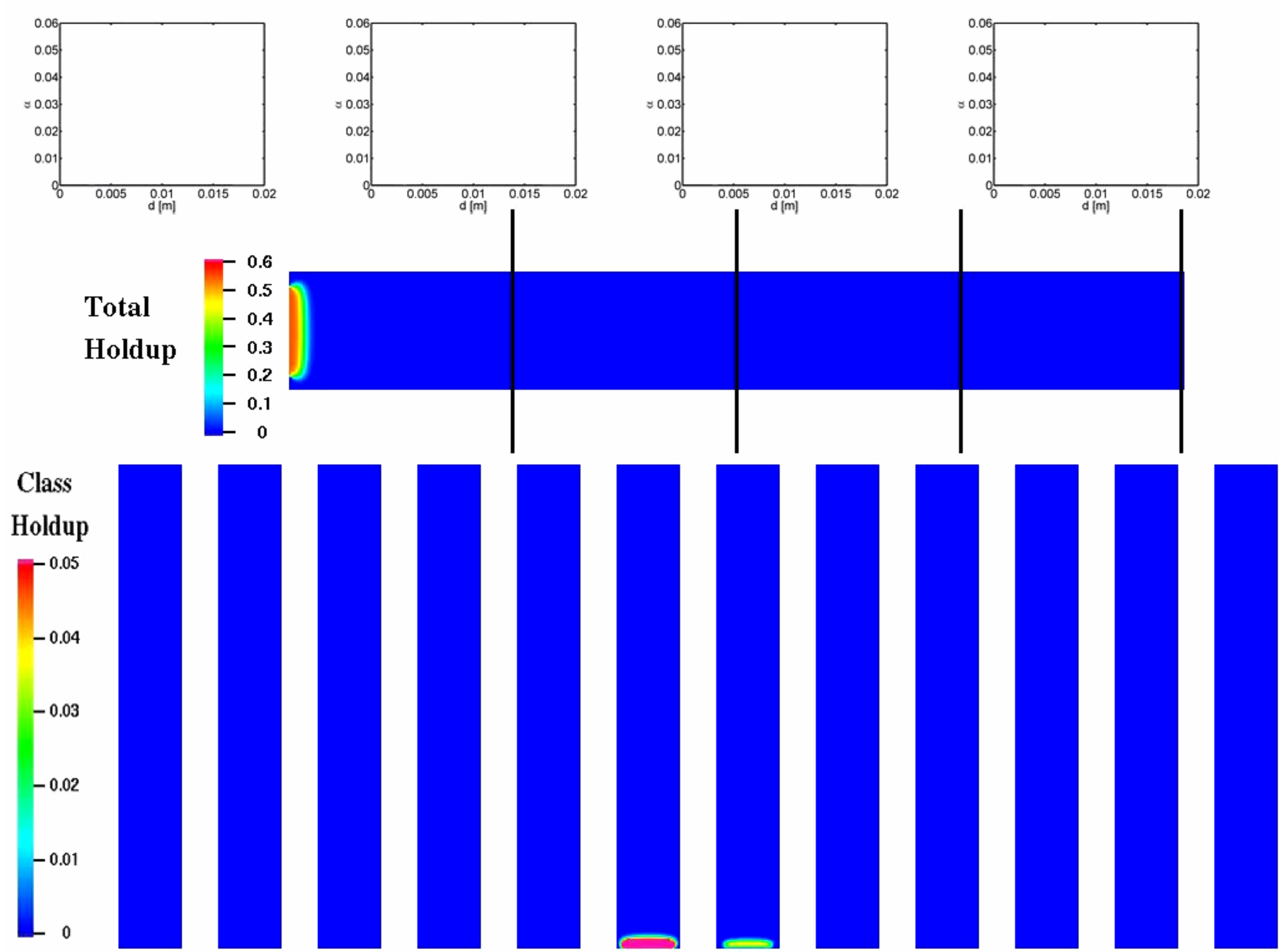
at t^n for a known f(d,**x**,t) with m parent class,

i. Calculate the source and sink terms due to coalescence and breakage at every $\mathbf{x}_i$ according to PPDC.
ii. With these calculated terms obtain the source and sink terms for first 2m order of moments.
iii. Convect the first 2m moments with these source and sink terms, solve 2m $\mathcal{C}$-$\mathcal{D}$ problem.
iv. Obtain the reduced PSD by product difference algorithm at every $\mathbf{x}_i$ which is f(d,**x**,t^{n+1}).



$$\left(M_L + \left(\theta K - B_i^- - C_i^-\right)\Delta t\right)\alpha_i^{\text{new}} = \left(M_L - \left(\left(1-\theta\right)K + B_i^+ + C_i^+\right)\Delta t\right)\alpha_i^{\text{old}}$$

Results: MC



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Class
Holdup
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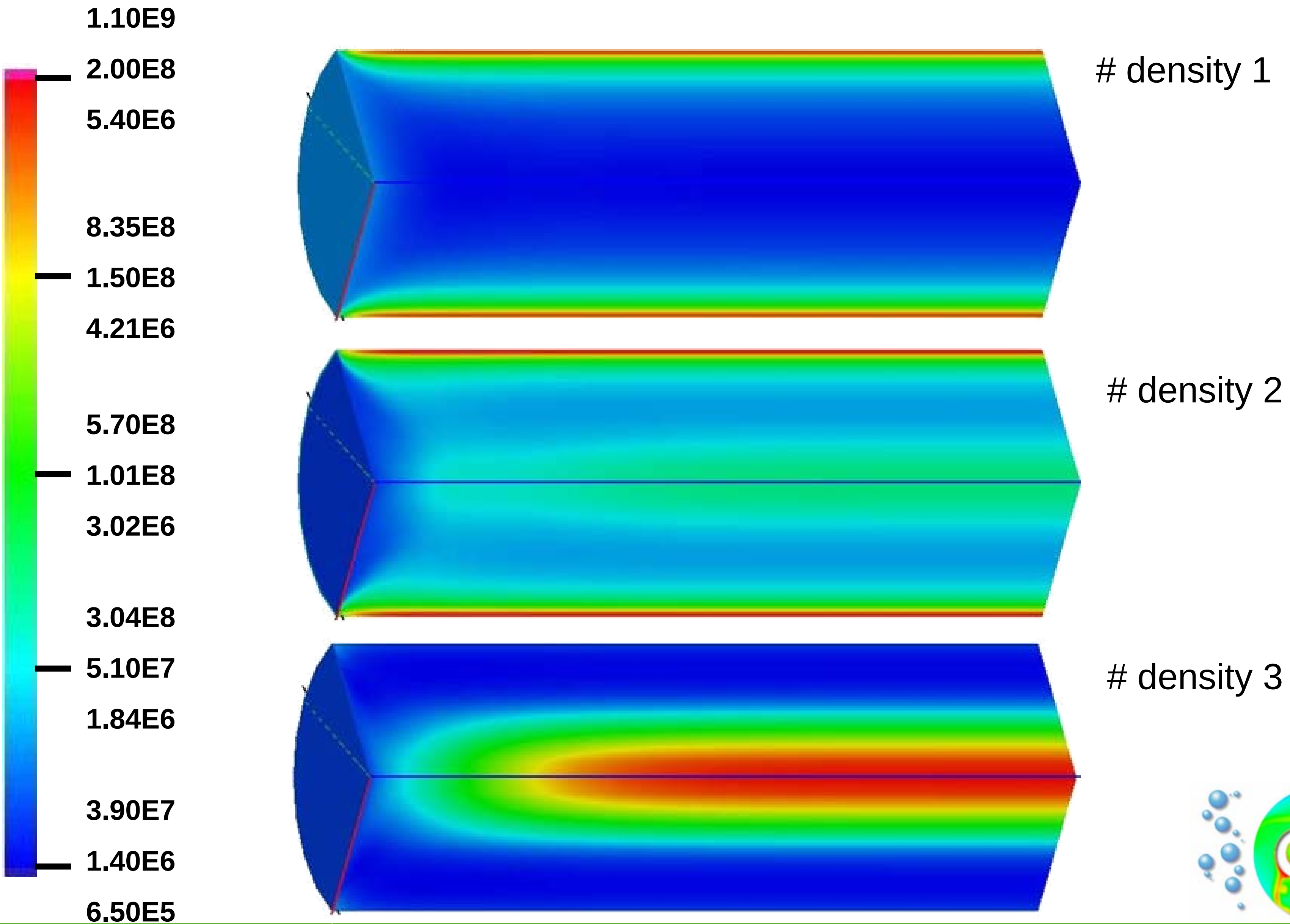
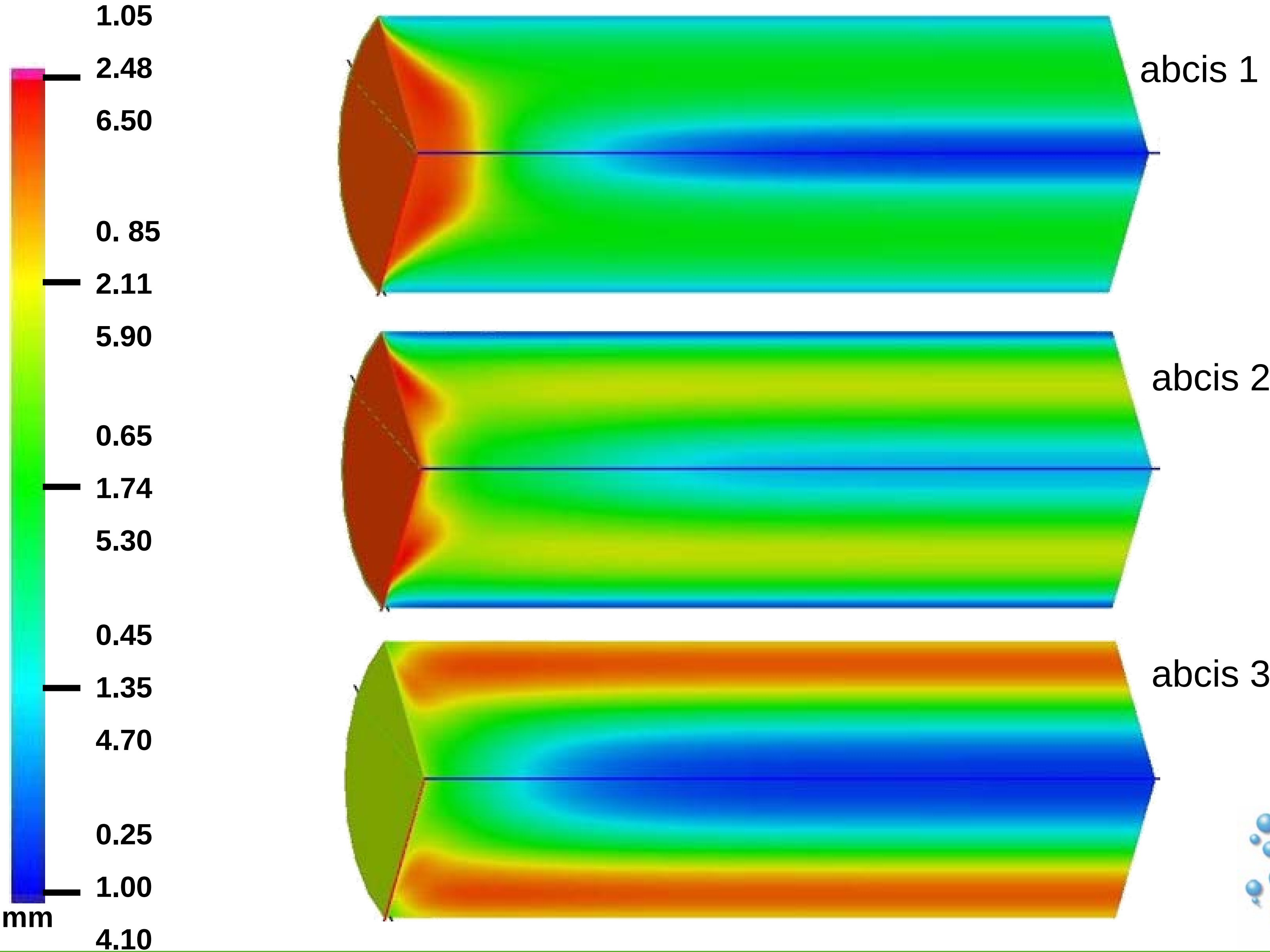
0.03
0.02
0.01
0

Results: PPDC number densities



Results: PPDC abcis



Results: PPDC moments

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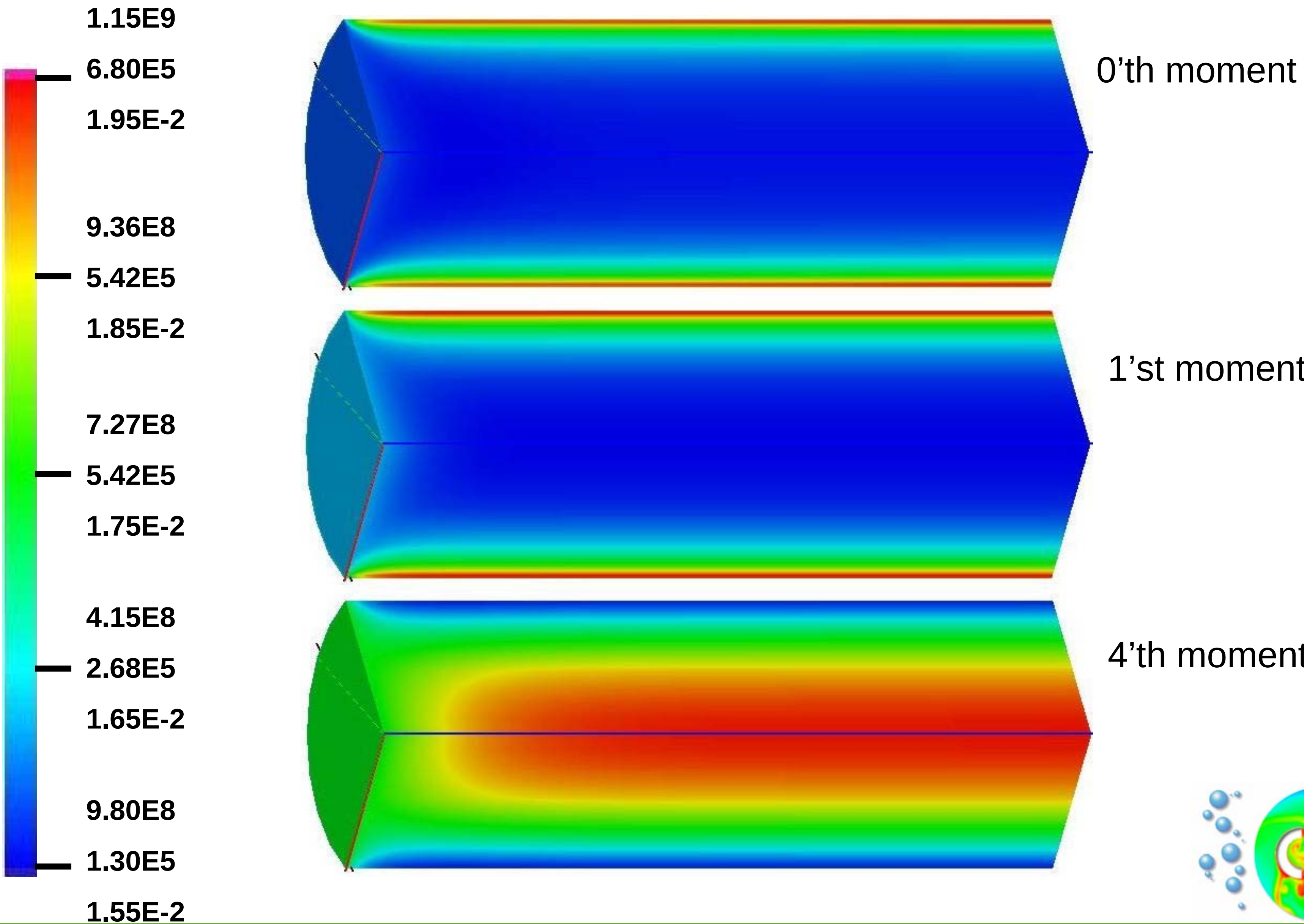
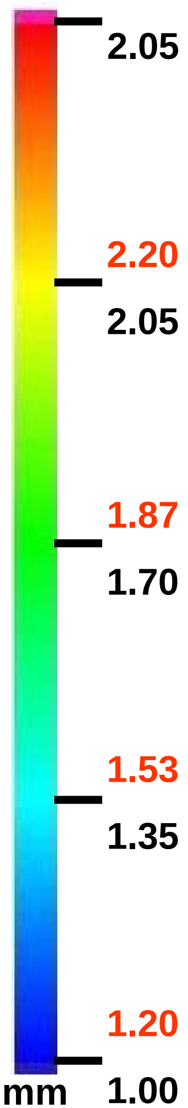
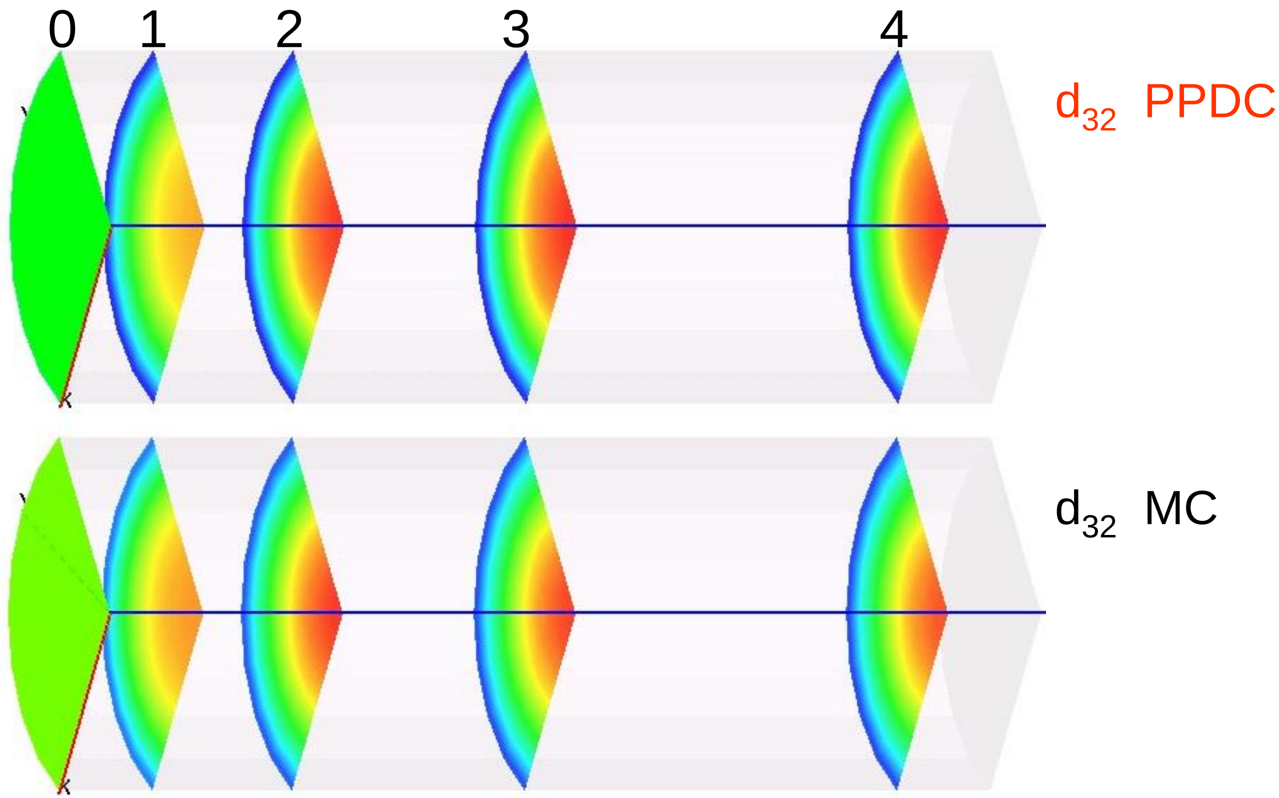


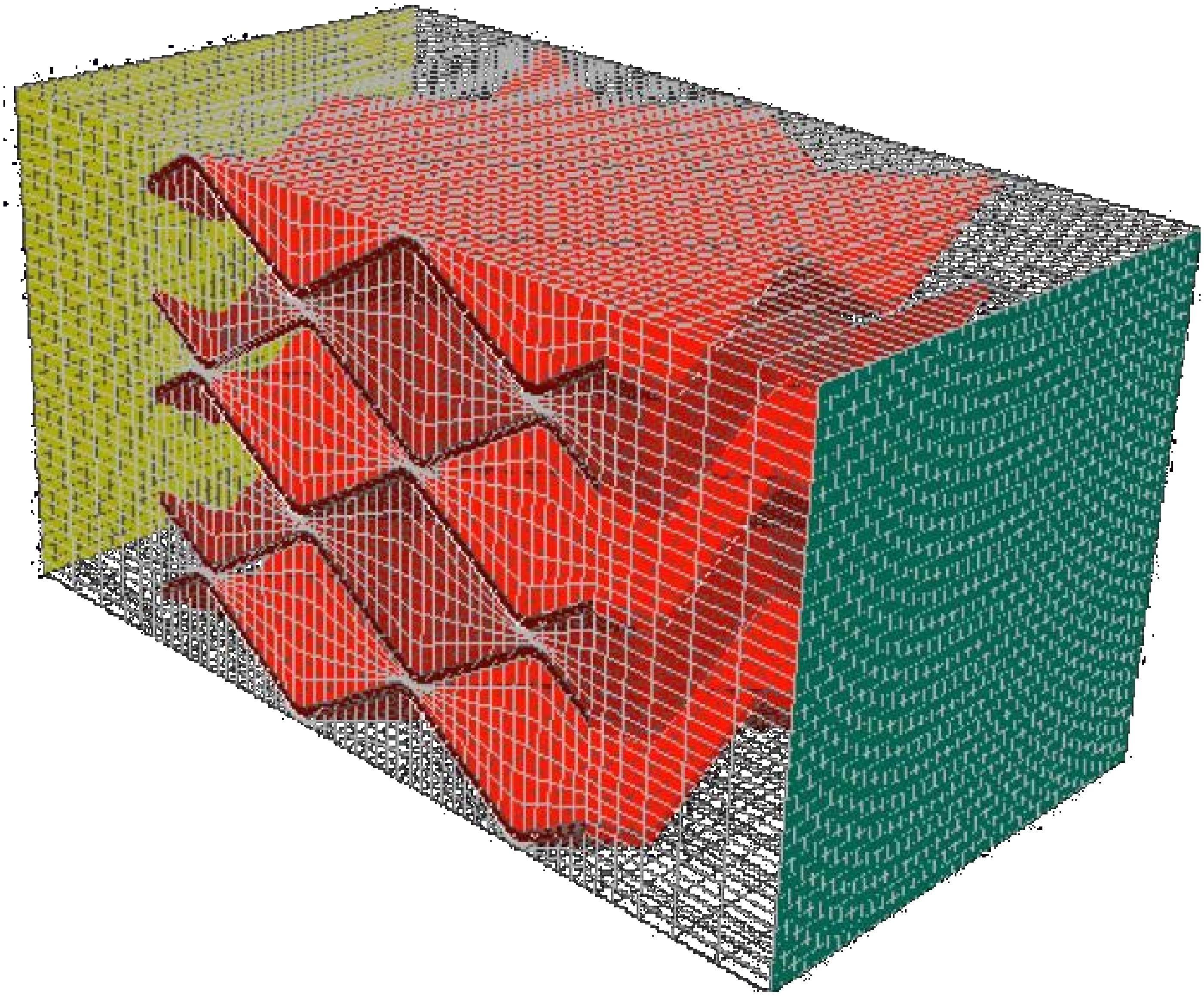
Results: PPDC vs MC



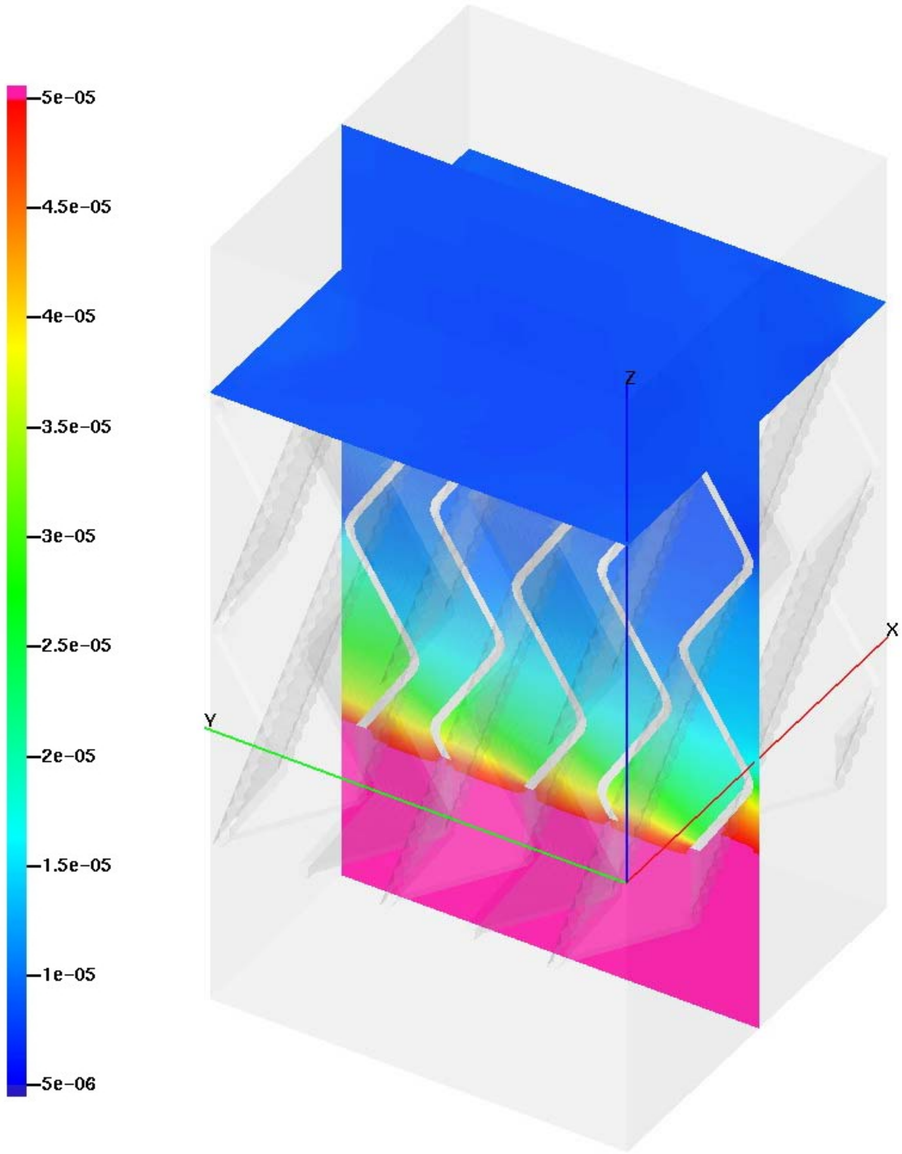


number density	4.9263e+008	5.4399e+008	5.5869e+008	5.6143e+008
	2.7821e+008	3.3381e+008	3.5106e+008	3.5366e+008
interfacial area density	1.0642e+003	1.0941e+003	1.1138e+003	1.1254e+003
	9.6713e+002	9.6144e+002	9.6379e+002	9.6448e+002
d_{32}	1.6914e-003	1.6451e-003	1.6160e-003	1.5994e-003
	1.8612e-003	1.8722e-003	1.8677e-003	1.8662e-003
d_{43}	2.8187e-003	2.6556e-003	2.5158e-003	2.4146e-003
	3.0212e-003	3.0824e-003	3.1032e-003	3.1045e-003

Results: Static Mixer

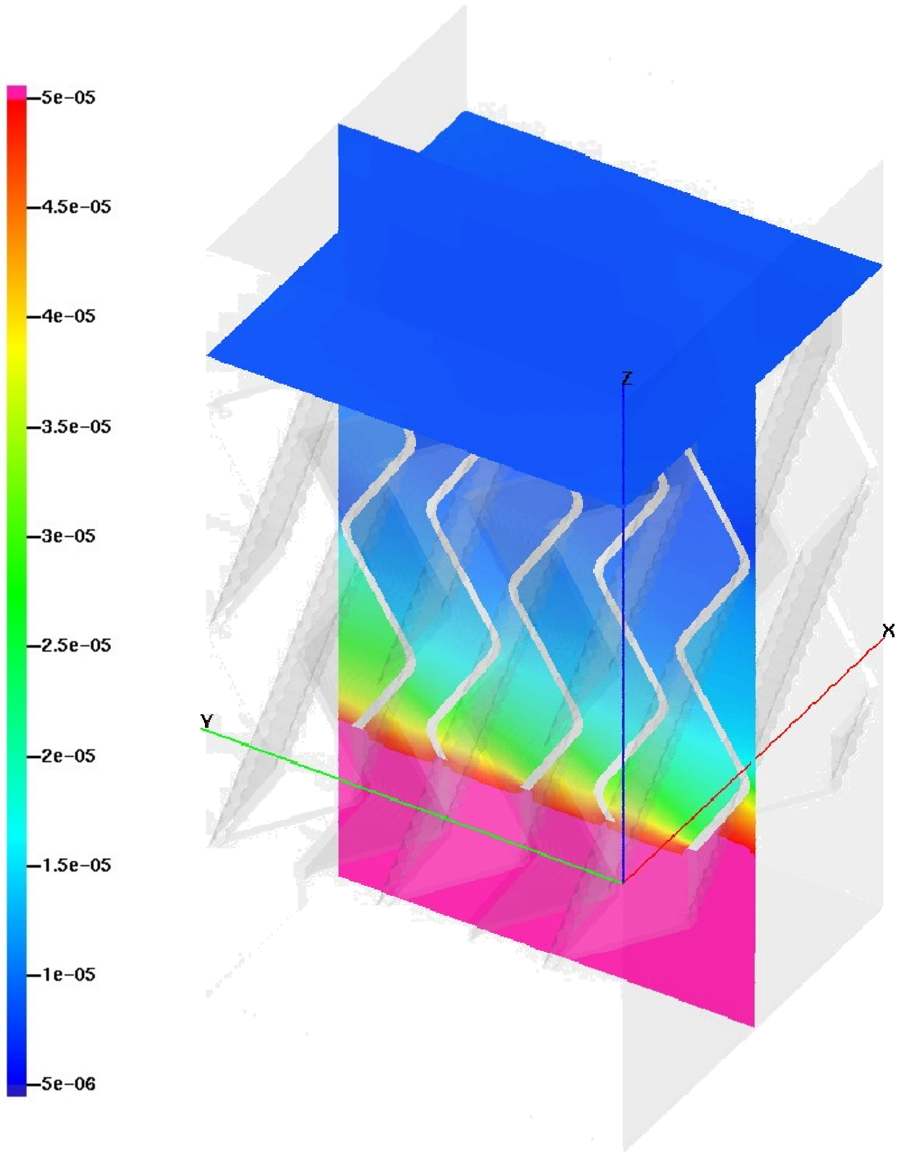


Results: Static Mixer



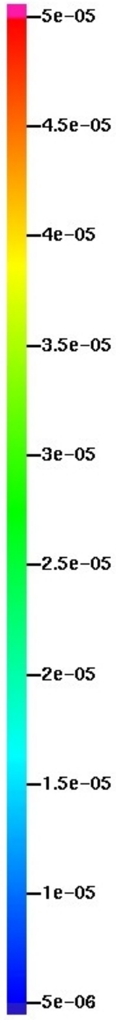
- xy plane at z=0.0219 m, distribution just after the mixer.
- yz plane is located at x = 0.0128 m, midplane in x.
- d_{32} = 10.55E-6 m

Results: Static Mixer

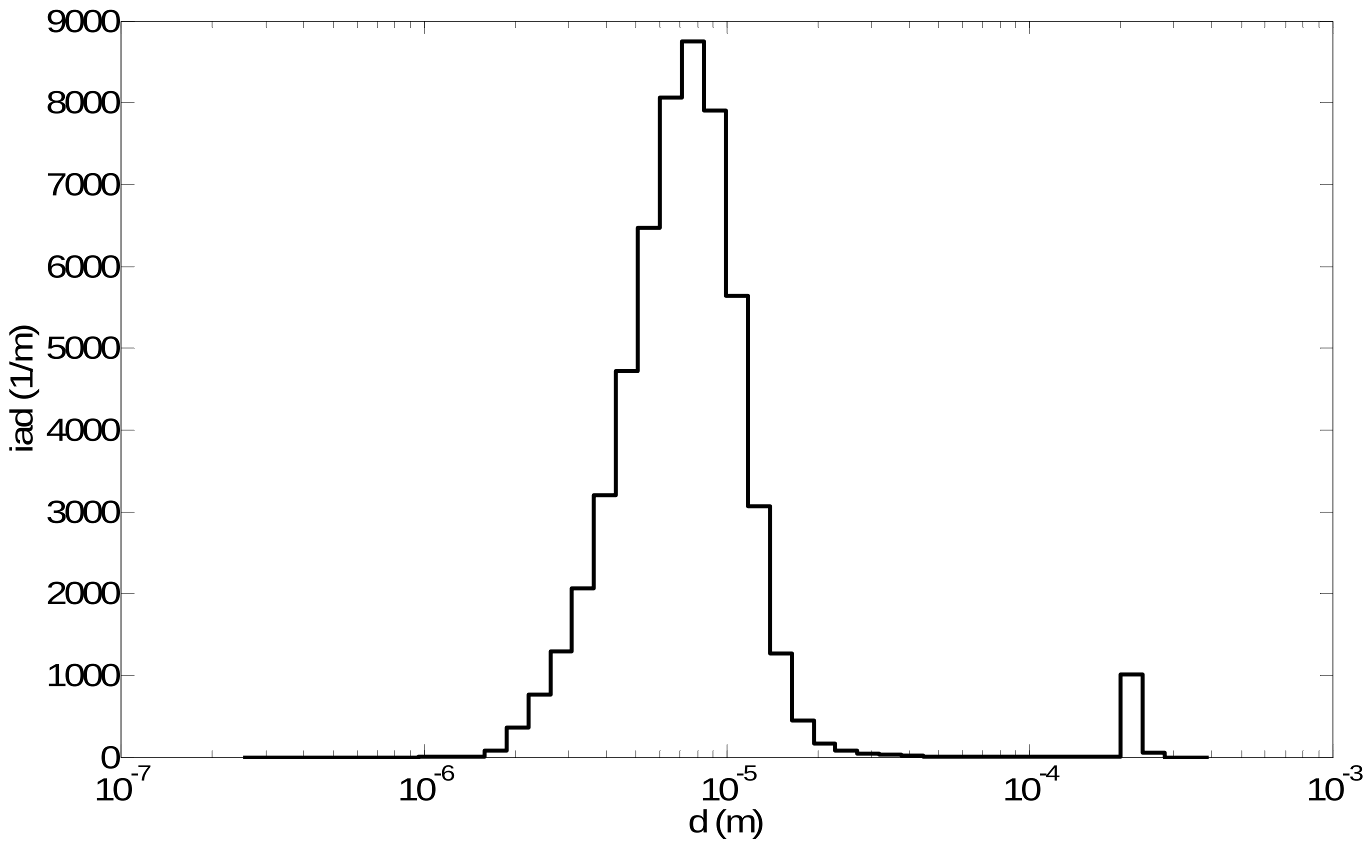


- xy plane at z=0.0243 m.
- d32 =10.63E-6 m.

Results: Static Mixer



- xy plane at z=0.0312 m, outlet.



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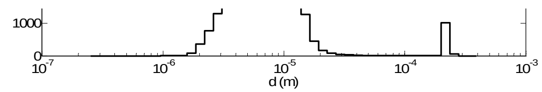
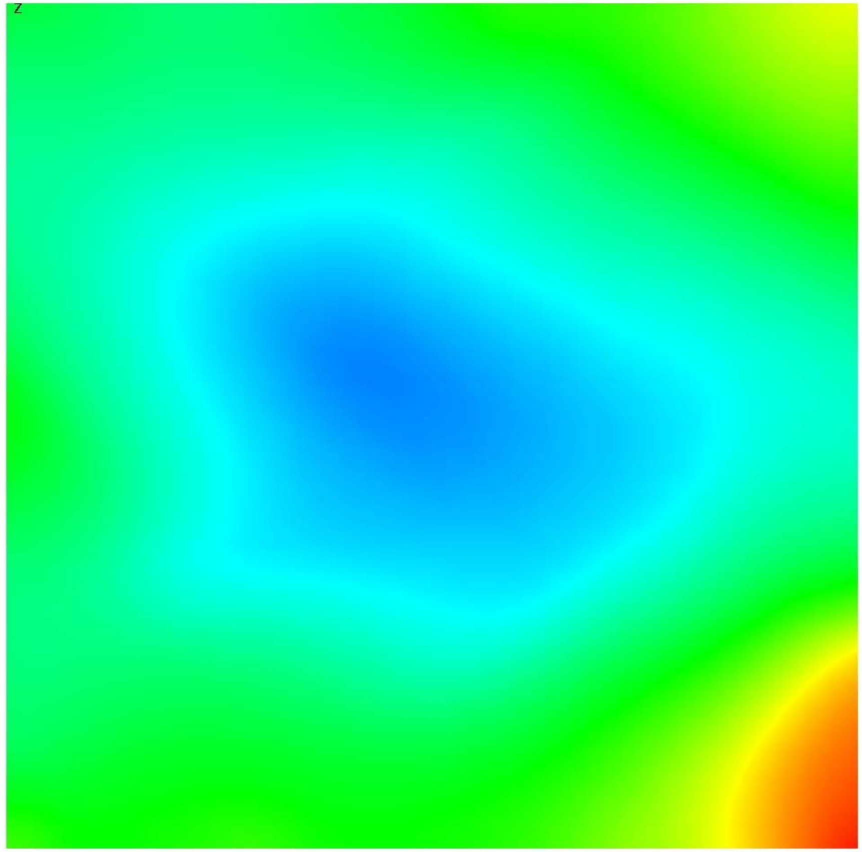


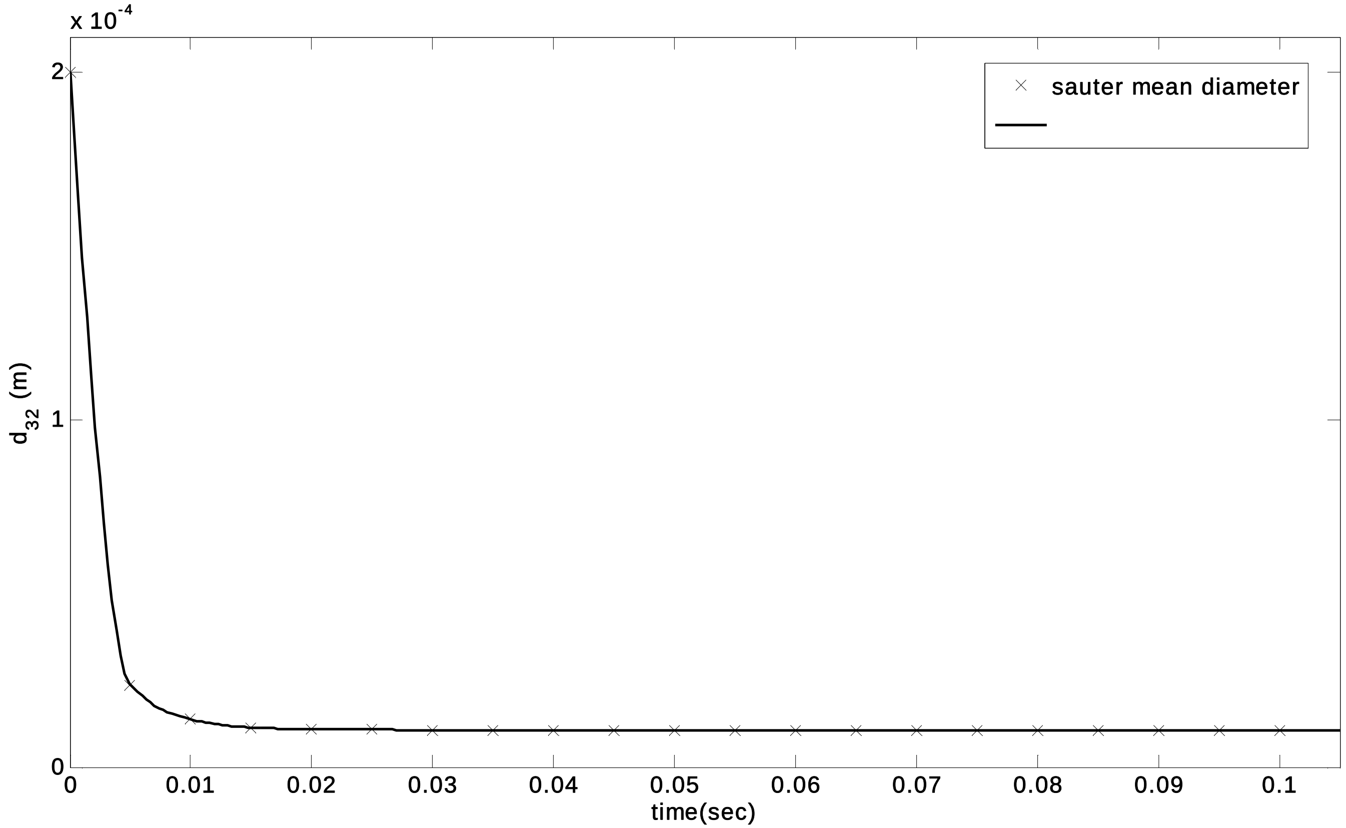
Results: Static Mixer

d_{32} distribution



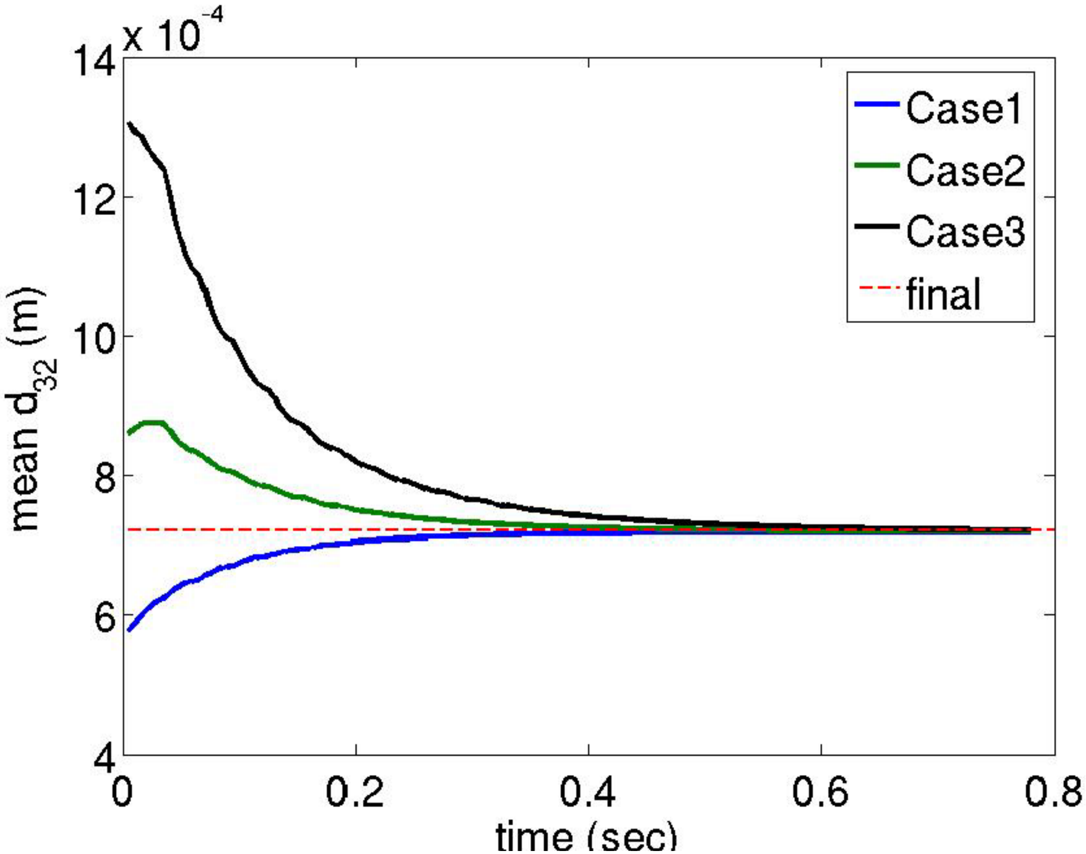
- 10.5E-6< d_{32}<11.2E-6, d_{32} = 10.8E-6 (all in meters)
- Dispersed phase is mixed homogenously in spatial space. Nevertheless, previous graphs has shown that mixing has a bimodal distribution.

Results: Static Mixer

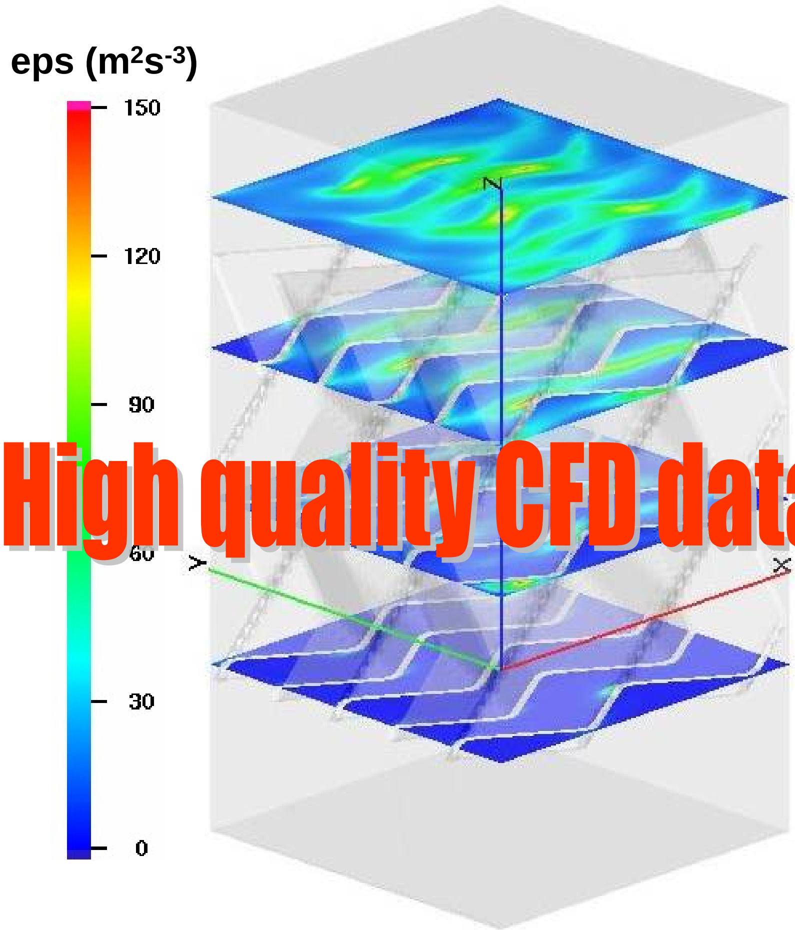


- Changes in the cutplanes are too small.
- After the first flow through (≈ 0.035 sec), d32 = 10.8E-6 m.

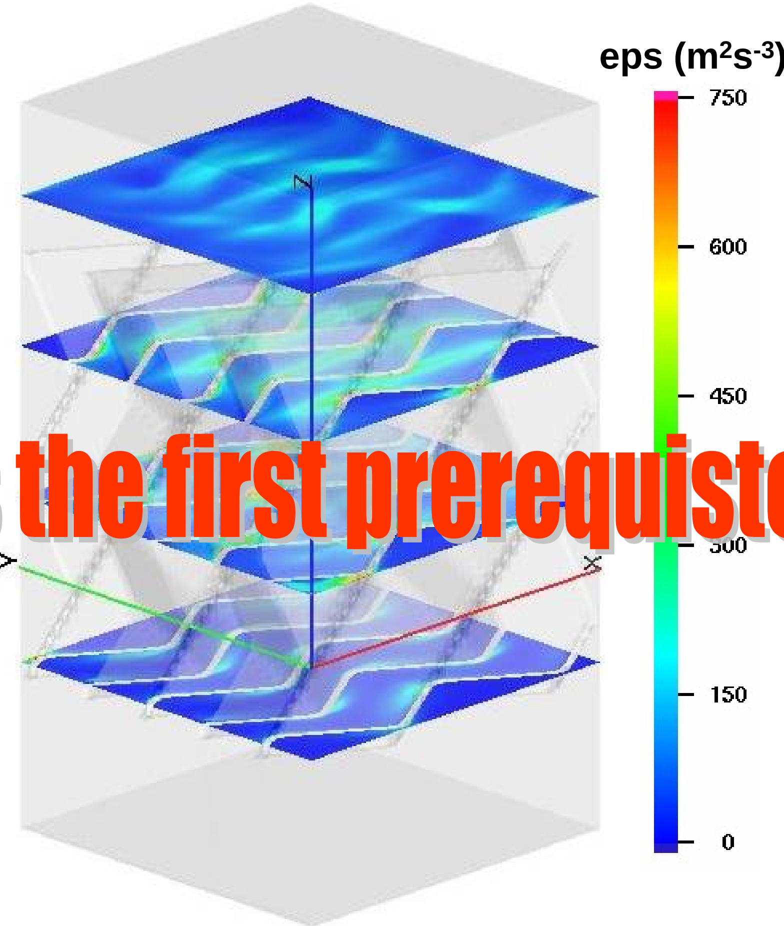
Results: Static Mixer



- Calculations for three different initial condition.
- d_{32} = 760E-6 m in equilibrium.
- d_{32} = 10.8E-6 m in equilibrium (recent).



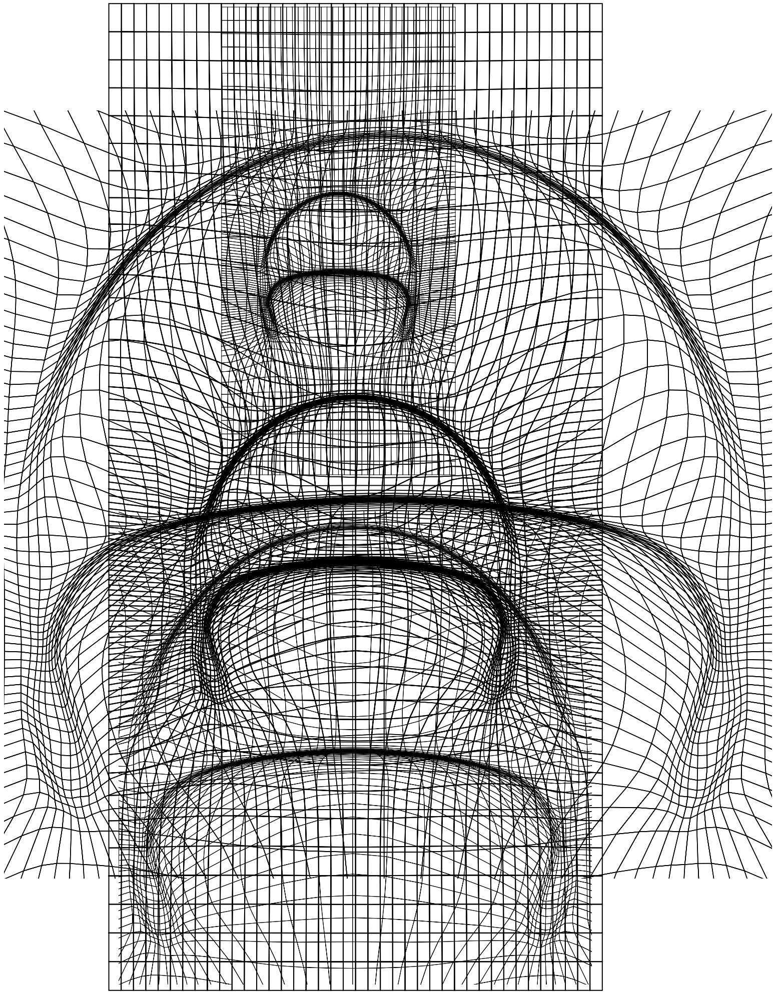
$d_{32} \approx 760E\text{-}6$ m

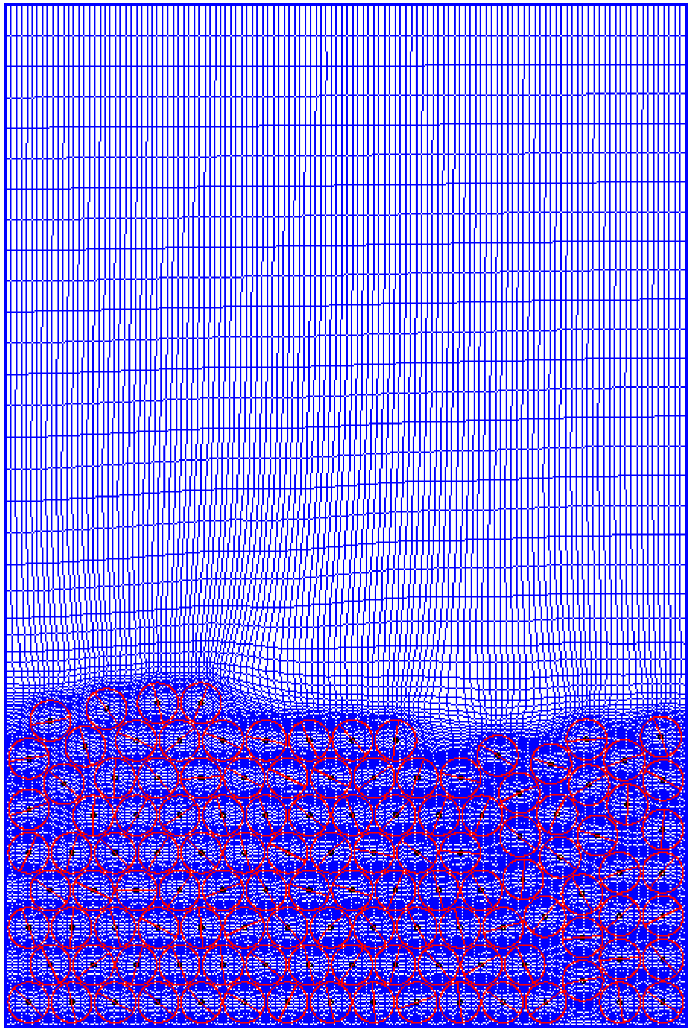


$d_{32} \approx 10.8E\text{-}6$ m

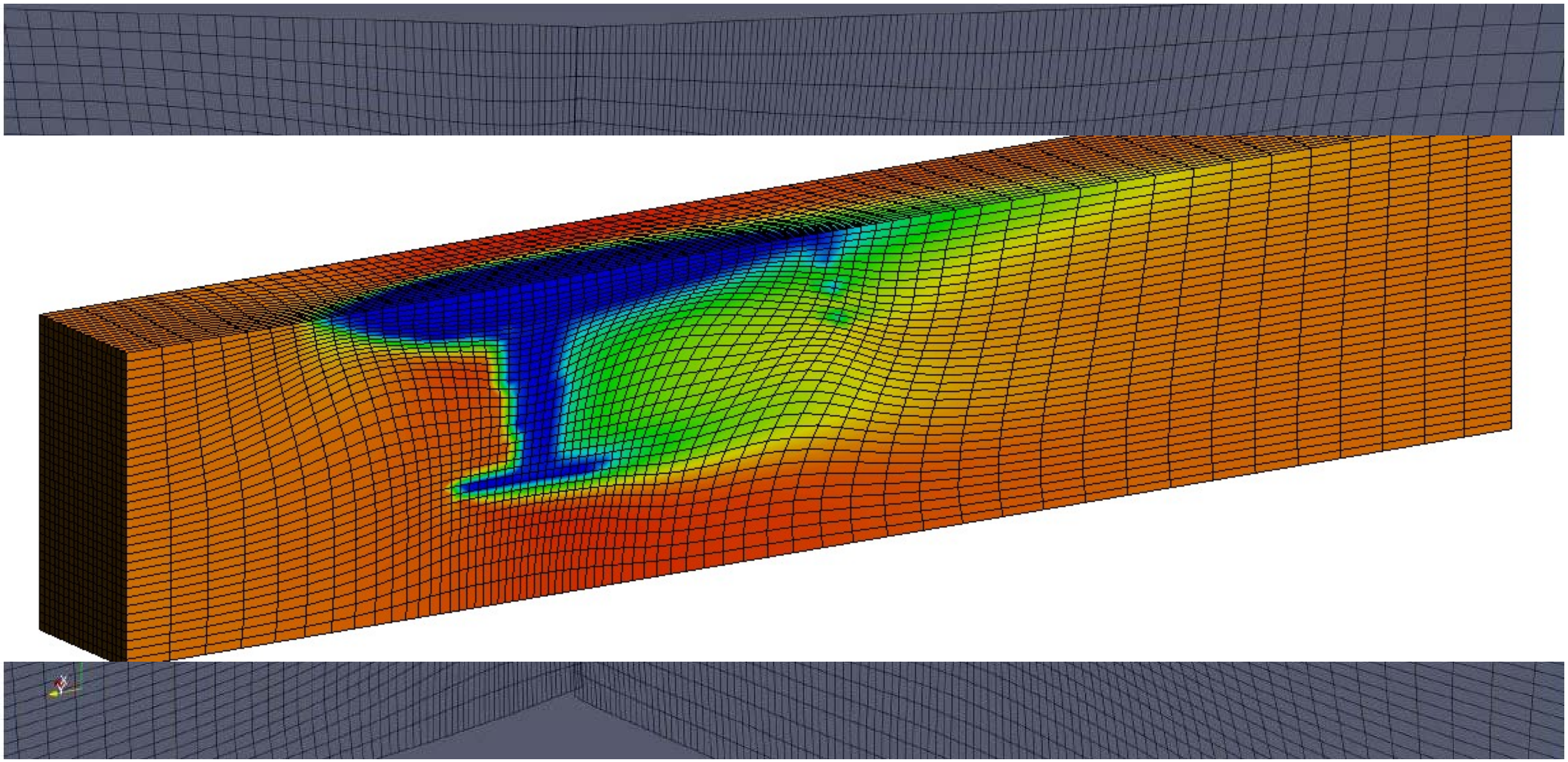
High quality CFD data is the first prerequiste!

Discussion: Mesh Deformation (2D)

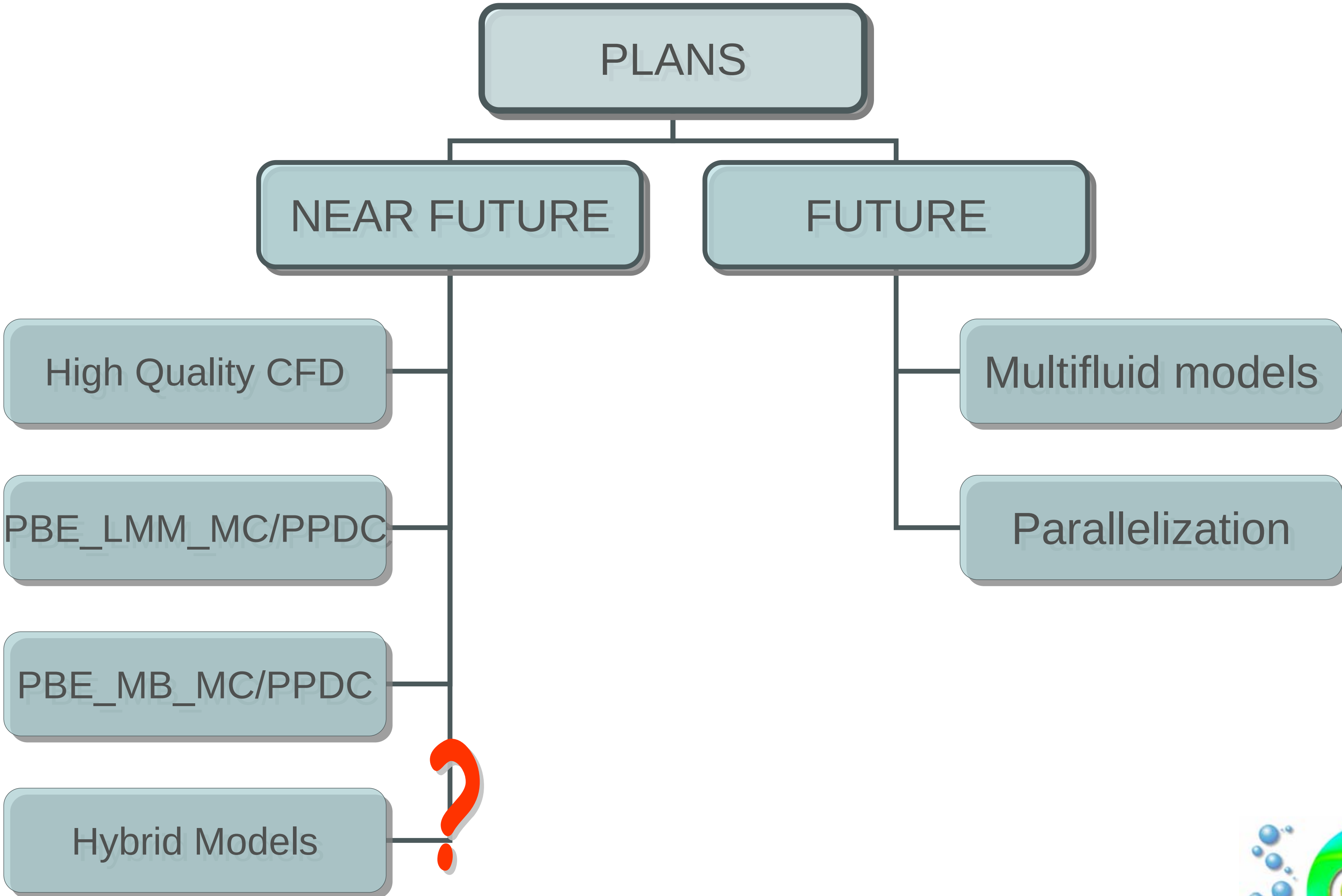




Discussion: Fictitious Boundary



Plans


PLANS
NEAR FUTURE
FUTURE
High Quality CFD
PBE_LMM_MC/PPDC
PBE_MB_MC/PPDC
Hybrid Models
?
Multifluid models
Parallelization

Thanks ...