Numerical Methods to Simulate Turbulent Dispersed Flows in Complex Geometries

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Stefan Turek

- **Introduction**
- **Governing Equations**
- **Population Balance Equations (PBEs)**
  - **Closure of PBEs**
    - **Breakage Kernel**
    - **Coalescence Kernel**
  - **Discretization of PBEs**
    - **Method of Classes**
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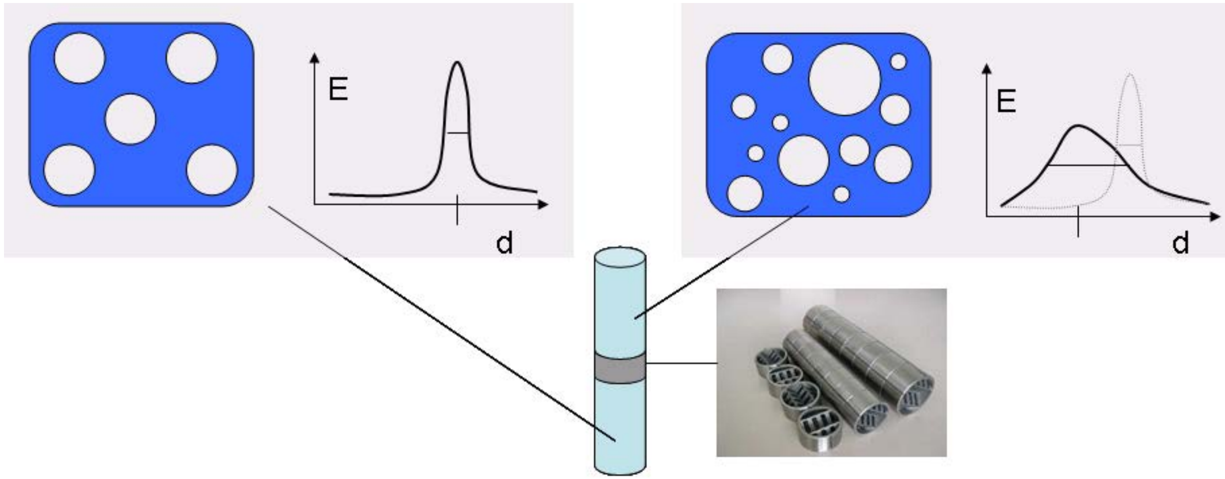
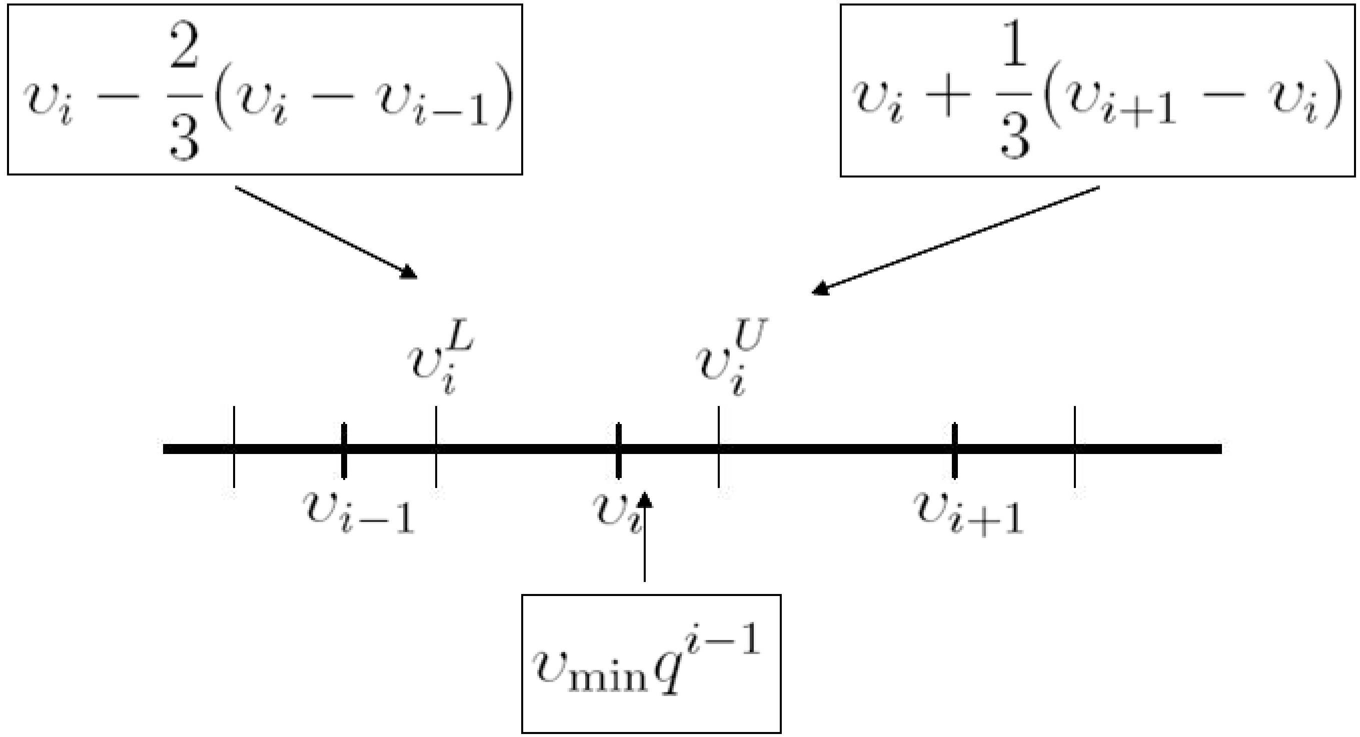
  - **Case Study: Sulzer Static Mixer, SMV™**
- **Fictitious Boundary Method**
  - **Packed Bed Reactor Simulations**
  - **Twin-Screw Simulations**
- **Outlook**



Evolution of the size distribution of the secondary phase

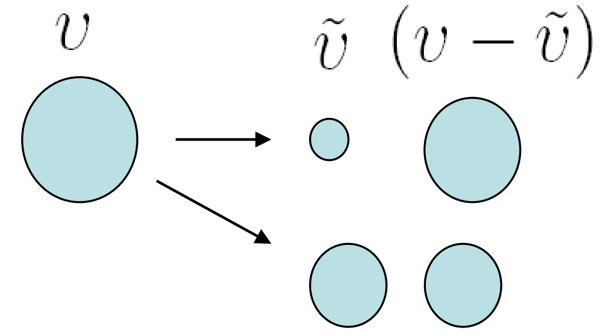
- IN
  - Time
  - Spatial coordinate
  - Internal coordinate
- WITH
  - Hydrodynamic variables
  - Physical properties

PBEs: Discretization

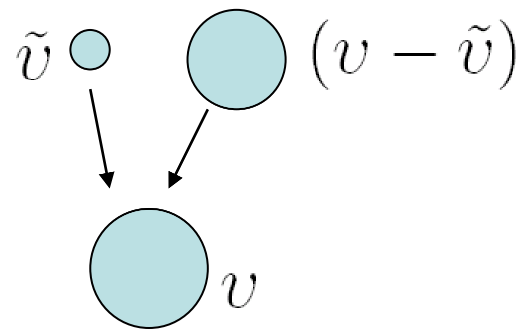


PBEs: Kernels

- Breakage Kernel
  1. F. Lehr & D. Mewes, 2001, CES
  2. V.V.Buwa & V.V.Ranade, 2002, CES
  3. F. Lehr *et al*., 2002, AIChe
  4. C. Martínez-Bazán *et al*., 1999, JFM
  5. T. Wang *et al*., 2003, CES



- Coalescence Kernel
  1. F. Lehr & D. Mewes, 2001, CES
  2. V.V.Buwa & V.V.Ranade, 2002, CES



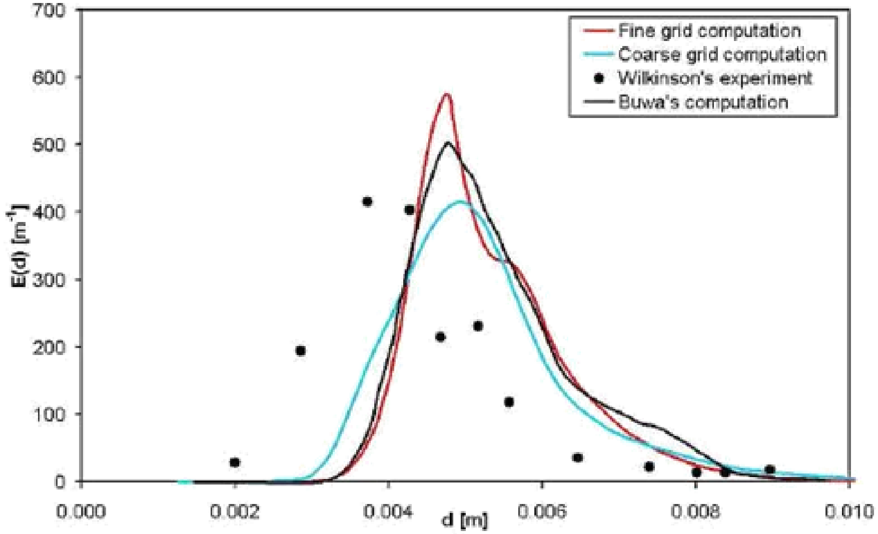
- Breakage Kernel

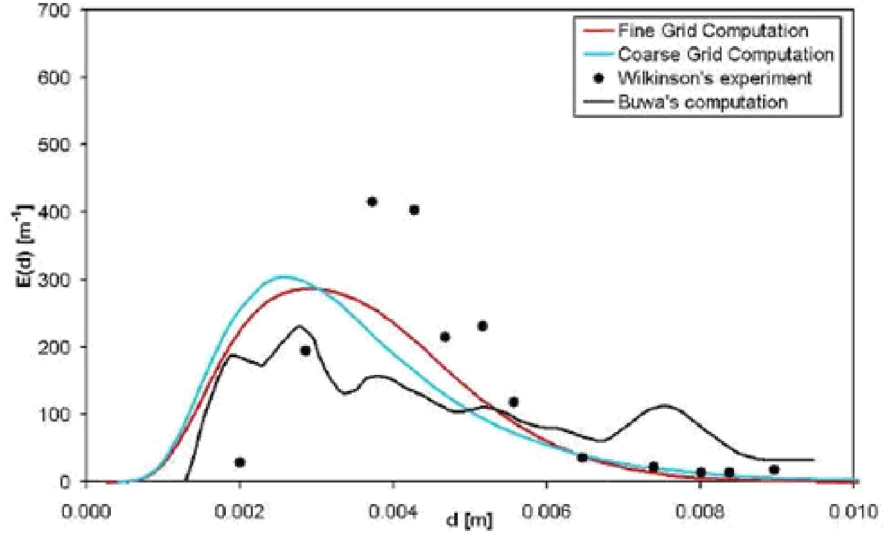
$$r^B(v,\tilde{v}) = K^B \Phi(v,\tilde{v}) \mathrm{in}(u', u_{\mathrm{crit}}), \quad u' = \sqrt{2}\varepsilon^{1/3}(d\tilde{d})^{1/6}$$

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

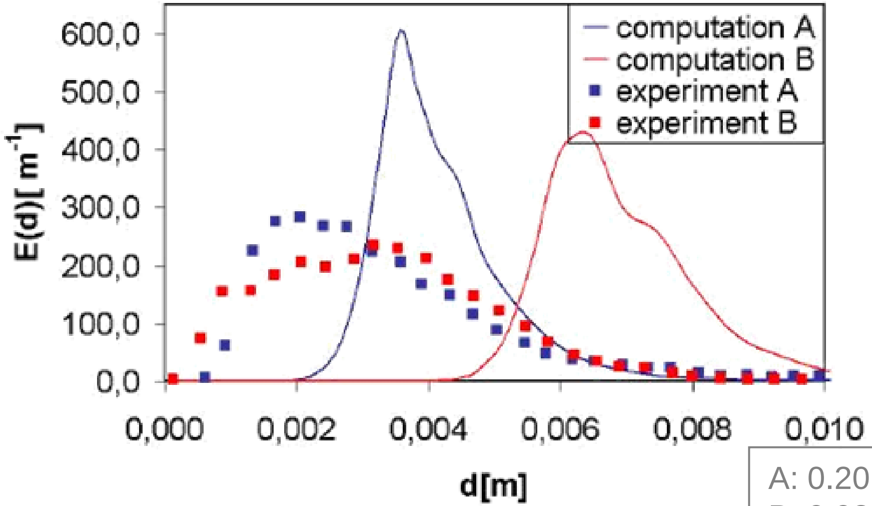
- $$\phi(v,\tilde{v}) = \frac{6}{\left(L\sqrt{\pi}\tilde{d}^*\right)^3} \frac{\exp\left(-2.25\left(\ln\left(2^{2/5}\tilde{d}^*\right)\right)^2\right)}{1+\mathrm{erf}\left(\ln\left(2^{1/15}d^*\right)^{1.5}\right)} \quad \text{for} \quad \tilde{v}^* \in (0, 0.5\rangle$$

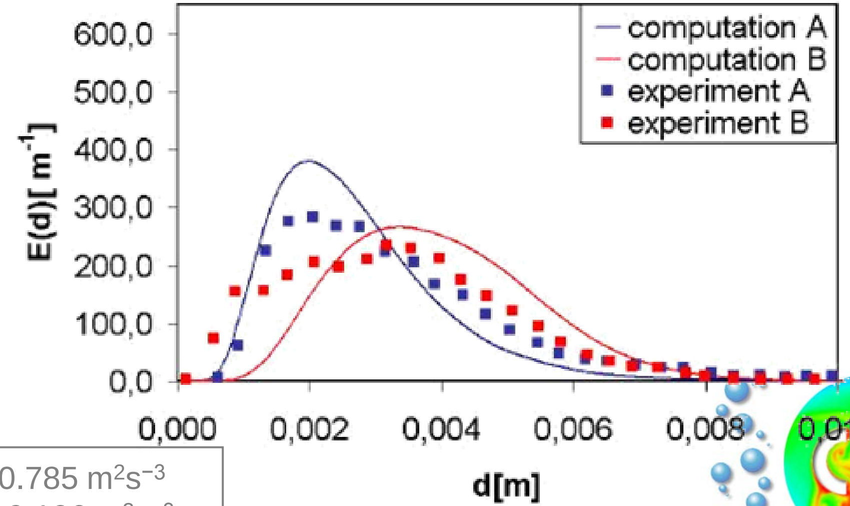
$$T = \left(\frac{\sigma}{\rho_L}\right)^{0.6} \frac{1}{\varepsilon^{0.4}} \quad \text{and} \quad L = \left(\frac{\sigma}{\rho_L}\right)^{0.4} \frac{1}{\varepsilon^{0.6}}$$





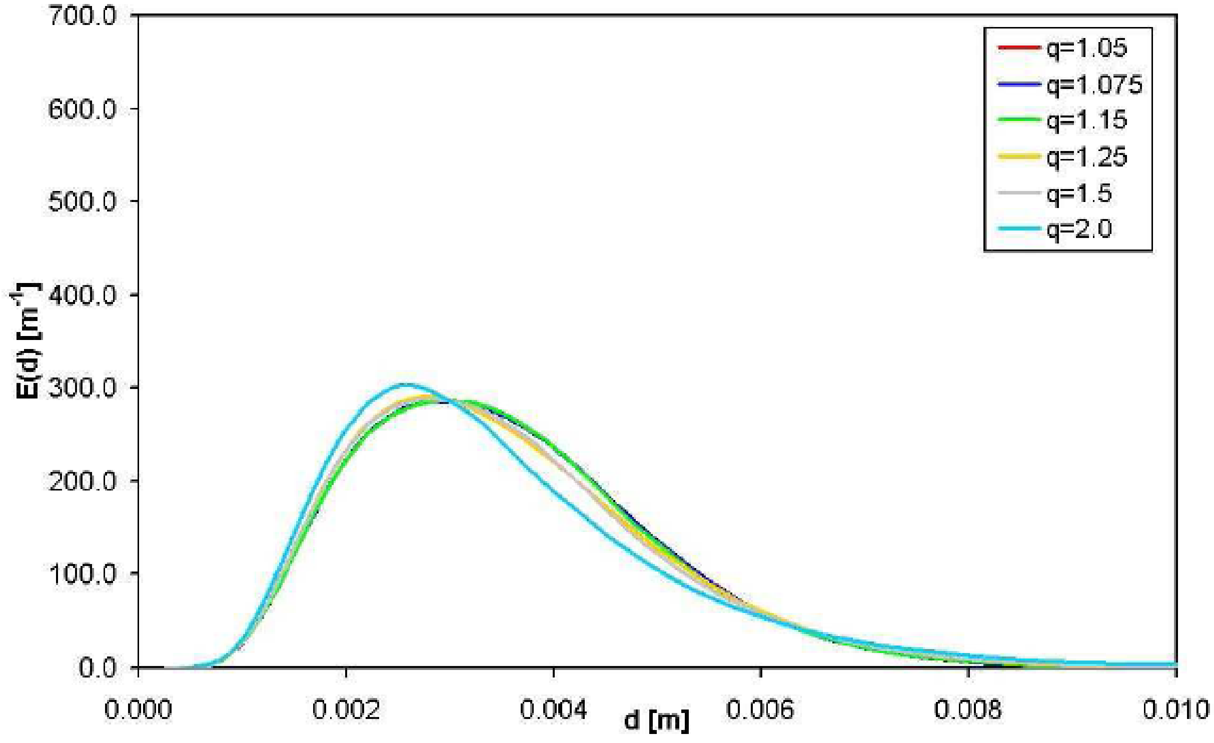
0.13; 0.3924 m^2s^{-3}





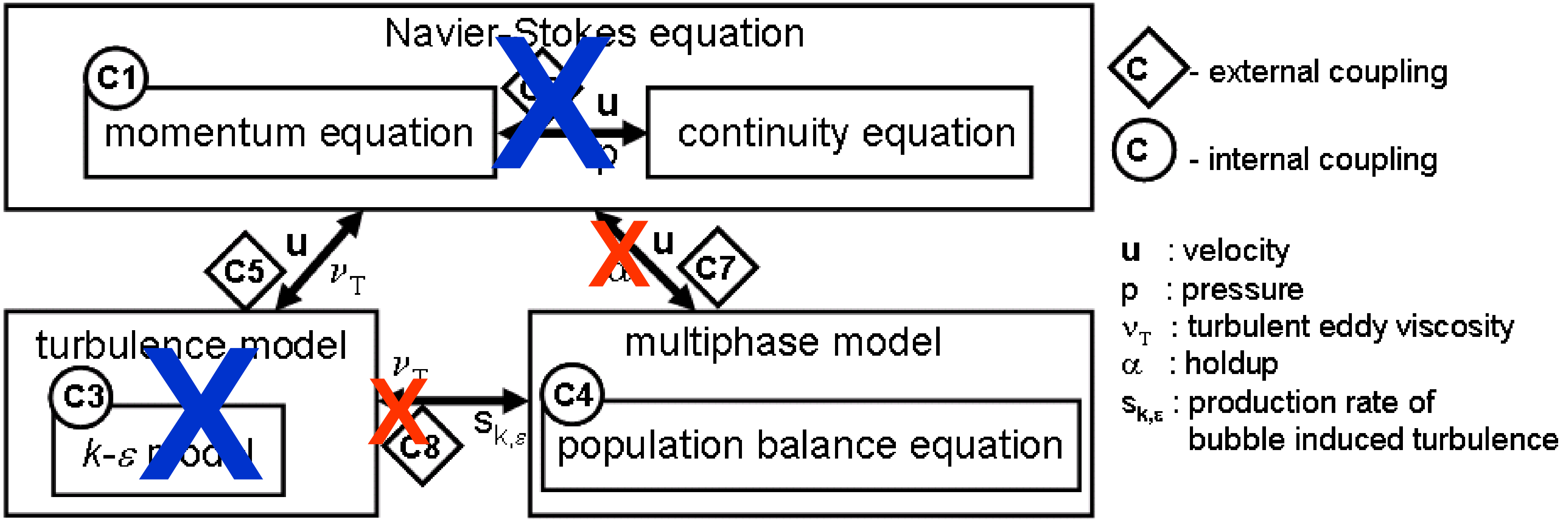
A: 0.20; 0.785 m^2s^{-3}
B: 0.08; 0.196 m^2s^{-3}

- Convergence behavior with discretization constant



Lehr et al., 2002

Non-stationary two way coupled, CFD - PBE.



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

Stationary one way coupled, CFD - PBE. X

One-way coupling

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

- High order discretization in time: fractional-step θ scheme, Crank-Nicolson
- Implicit treatment of sink terms results in positivity preserving schemes
- High order spatial discretization is achieved by TVD scheme.

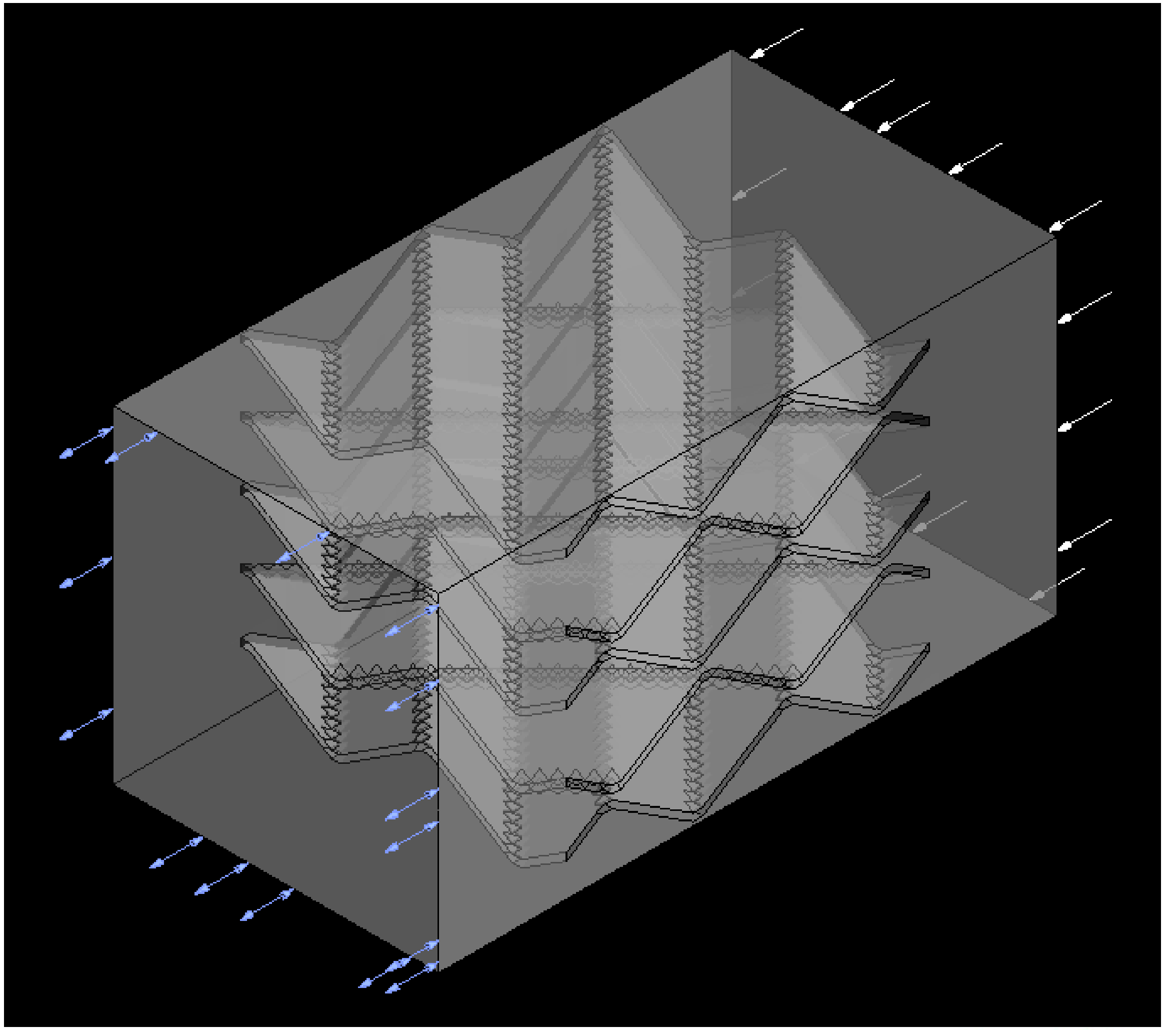
$$\left(M_L + \left(\theta(K+S) - B_i^- - C_i^-\right) \Delta t\right) \alpha_i^{\text{new}} =$$
$$\left(M_L - \left((1-\theta)\,(K+S) + B_i^+ + C_i^+\right) \Delta t\right) \alpha_i^{\text{old}}$$

- Defect correction loop

$$A(\mathbf{u}^{(n)}, \nu_T^{(n)}, B_i^{\pm(l)}, C_i^{\pm(l)}) \Delta\alpha_i^{(m+1)} = r^{(m)}$$
$$\alpha_i^{(m+1)} = \alpha_i^{(m)} + \omega \Delta\alpha_i^{(m+1)}$$

Our industrial partners

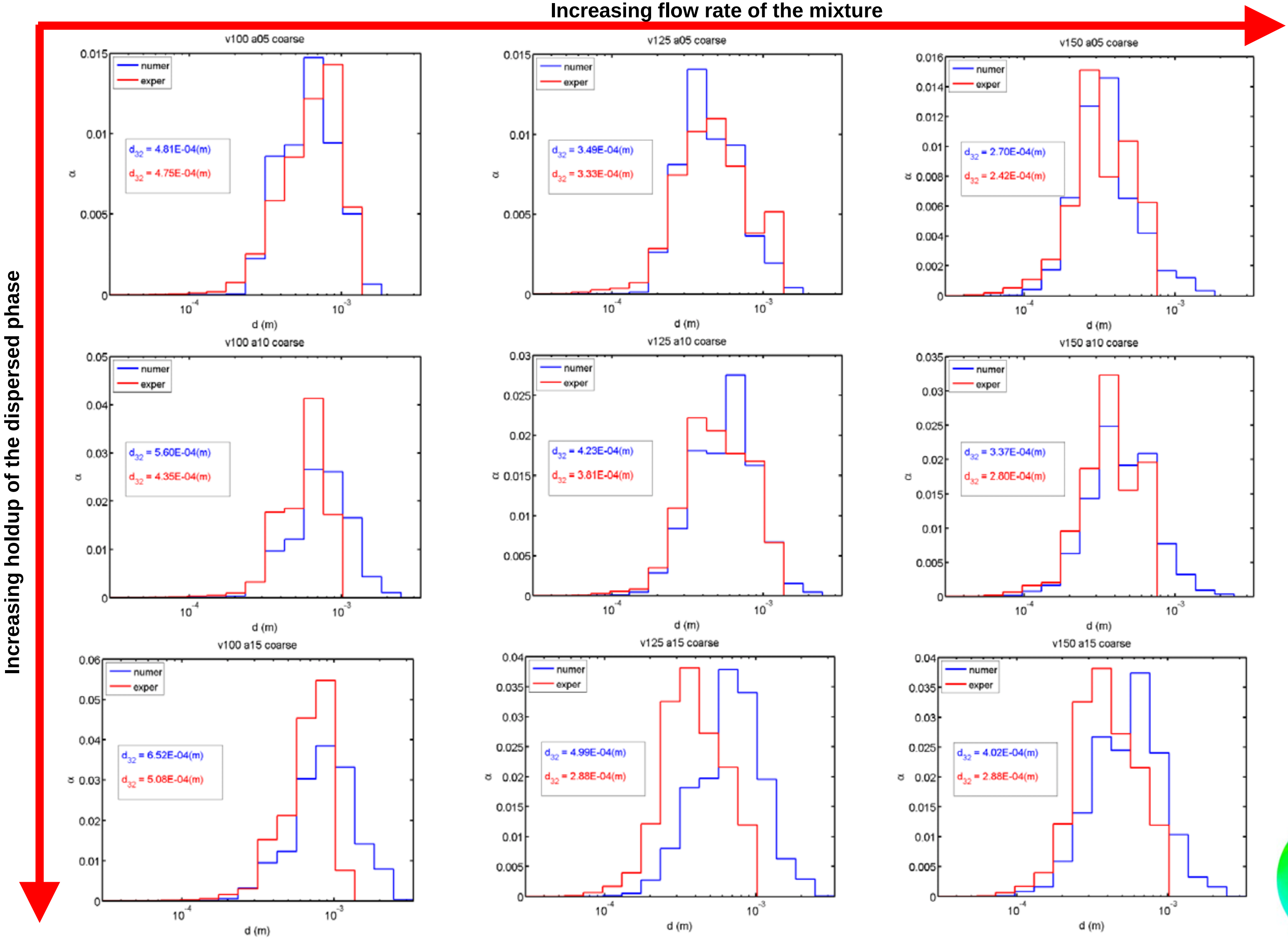
- **Sulzer ChemTech**
- **Sulzer Innotec**



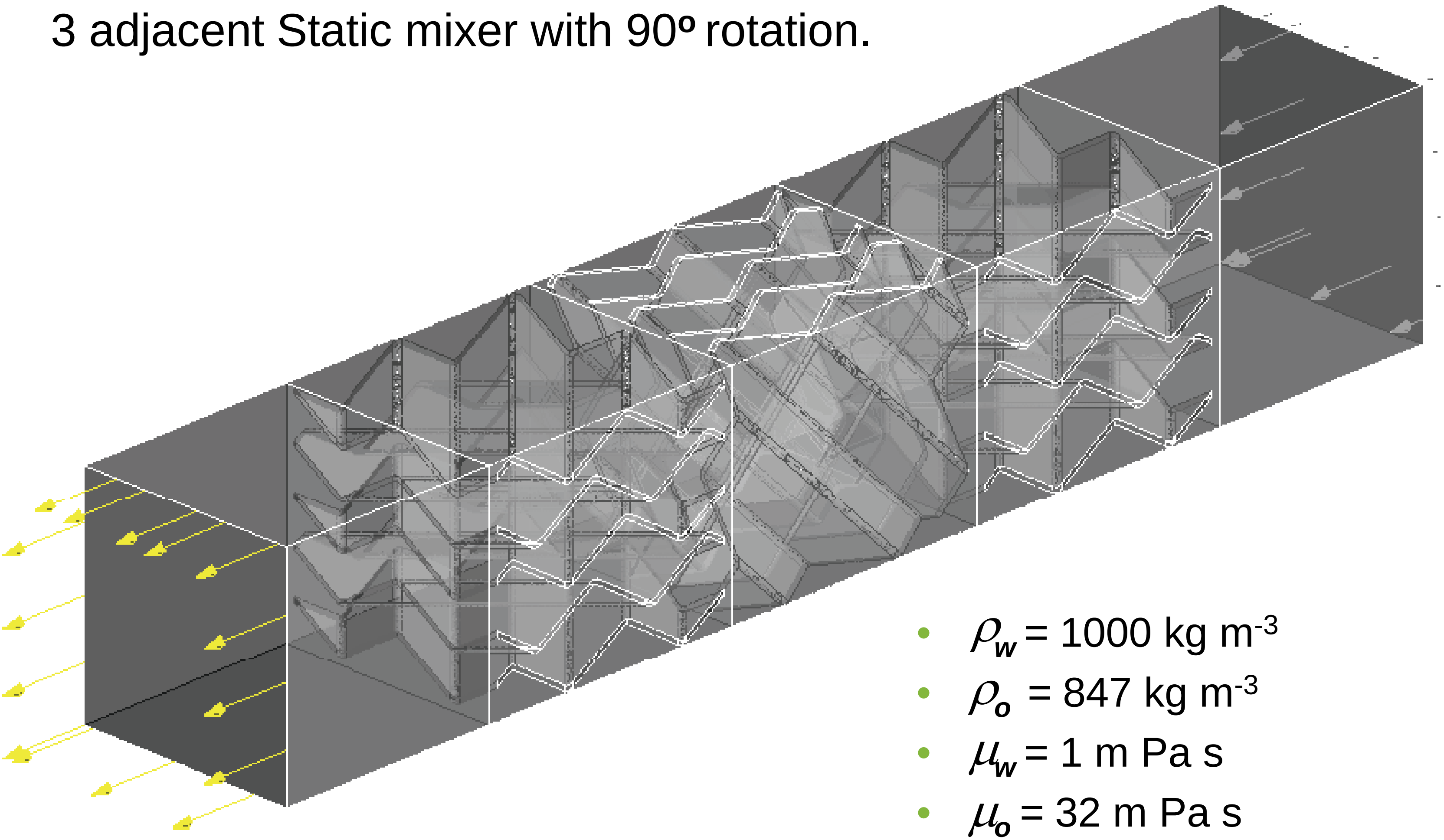
Physical Properties

- $\rho_w = 1000$ kg m^{-3}
- $\rho_o = 847$ kg m^{-3}
- $\mu_w = 1$ mPa s
- $\mu_o = 32$ mPa s
- $\sigma_{ow} = 0.043$N m^{-1}

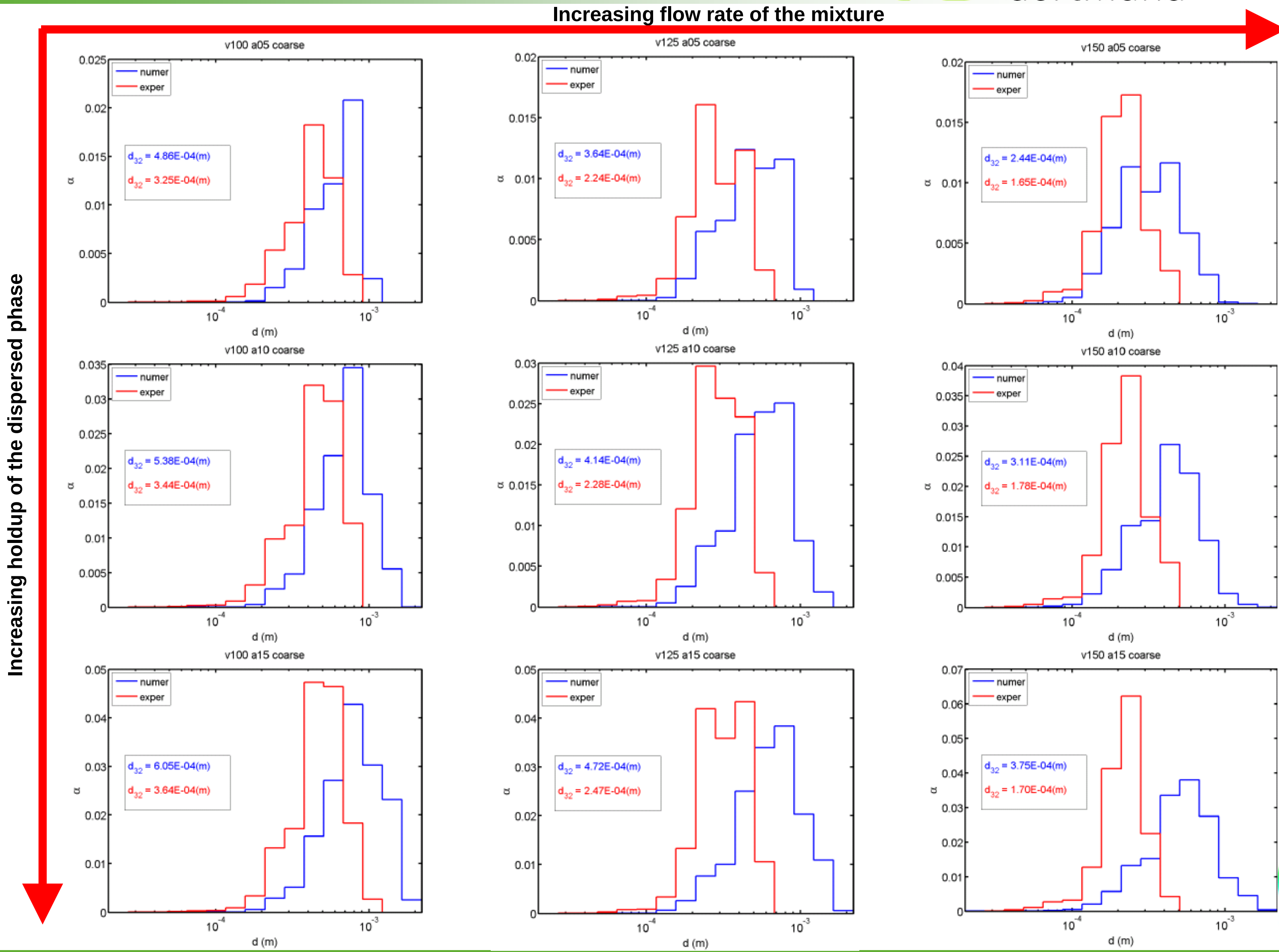
Sulzer, 1 SMV™


Increasing flow rate of the mixture
Increasing holdup of the dispersed phase
v100 a05 coarse
numer
exper
d32 = 4.81E-04(m)
d32 = 4.75E-04(m)
v125 a05 coarse
d32 = 3.49E-04(m)
d32 = 3.33E-04(m)
v150 a05 coarse
d32 = 2.70E-04(m)
d32 = 2.42E-04(m)
v100 a10 coarse
d32 = 5.60E-04(m)
d32 = 4.35E-04(m)
v125 a10 coarse
d32 = 4.23E-04(m)
d32 = 3.81E-04(m)
v150 a10 coarse
d32 = 3.37E-04(m)
d32 = 2.80E-04(m)
v100 a15 coarse
d32 = 6.52E-04(m)
d32 = 5.08E-04(m)
v125 a15 coarse
d32 = 4.99E-04(m)
d32 = 2.88E-04(m)
v150 a15 coarse
d32 = 4.02E-04(m)
d32 = 2.88E-04(m)
α
d (m)

3 adjacent Static mixer with 90º rotation.



- ρ_w = 1000 kg m^{-3}
- ρ_o = 847 kg m^{-3}
- μ_w = 1 m Pa s
- μ_o = 32 m Pa s
- σ_{ow} = 0.043N m^{-1}


Increasing flow rate of the mixture
Increasing holdup of the dispersed phase
v100 a05 coarse
numer
exper
d32 = 4.86E-04(m)
d32 = 3.25E-04(m)
v125 a05 coarse
d32 = 3.64E-04(m)
d32 = 2.24E-04(m)
v150 a05 coarse
d32 = 2.44E-04(m)
d32 = 1.65E-04(m)
v100 a10 coarse
d32 = 5.38E-04(m)
d32 = 3.44E-04(m)
v125 a10 coarse
d32 = 4.14E-04(m)
d32 = 2.28E-04(m)
v150 a10 coarse
d32 = 3.11E-04(m)
d32 = 1.78E-04(m)
v100 a15 coarse
d32 = 6.05E-04(m)
d32 = 3.64E-04(m)
v125 a15 coarse
d32 = 4.72E-04(m)
d32 = 2.47E-04(m)
v150 a15 coarse
d32 = 3.75E-04(m)
d32 = 1.70E-04(m)
d (m)
α

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Fluid simulation with complex geometries:

- Eulerian approach
  - ► Use a fixed grid (no need for remeshing)
  - ► Improve boundary approximation by grid adaptation

FBM-Algorithm:

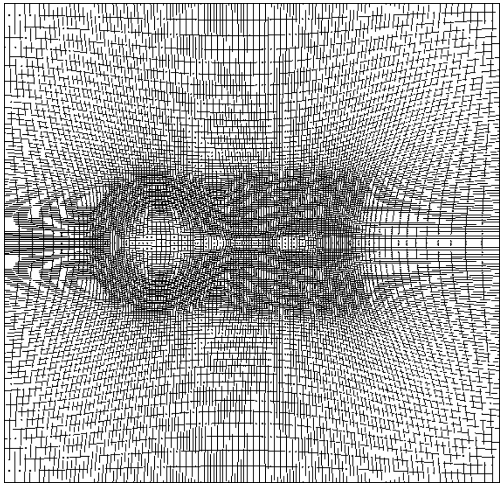
- Identify the DOFs inside the geometry (*point location problem*)
- Replace corresponding matrix rows with rows of the identity matrix
- Prescribe dirichlet values in the RHS

Efficient solution of point location problem:

- Domain Decomposition
- Geometrical Multigrid: Hierarchical mesh structure (Bounding Volume Hierarchies)

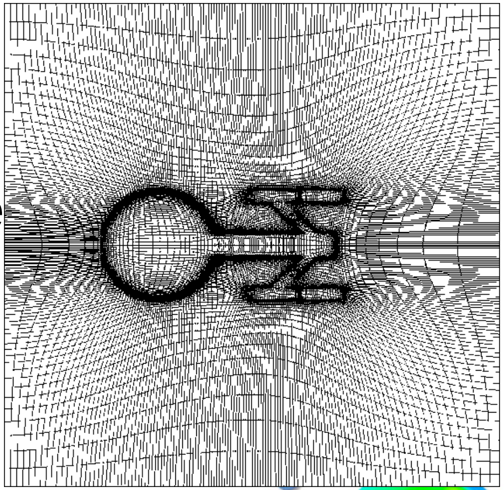
Idea :

- Describe desired vertex positions in terms of cell size
  - ► Small cell sizes → high vertex concentration
- *Monitor function*: user-defined cell size distribution
- Use distance functions or error-distribution functions

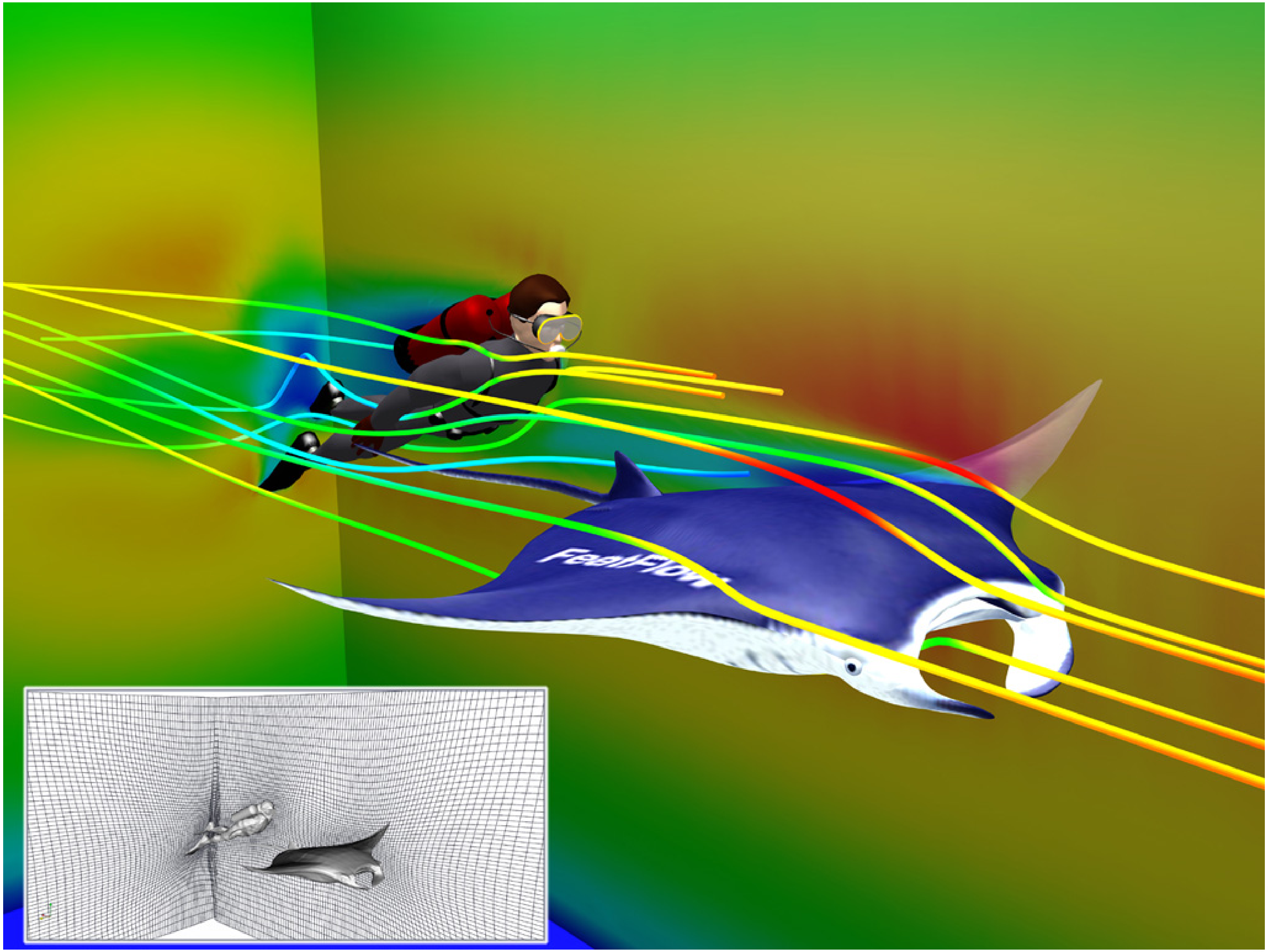


Numerical Realization:

- Poisson problem with relative cell size change as RHS
- Recover the gradient of the resulting scalar field
  - ► Velocity field along which the vertices should move
- Numerically integrate the velocity in the vertices
  - ►New vertex positions



Grid deformation preserves the (local) logical structure of the grid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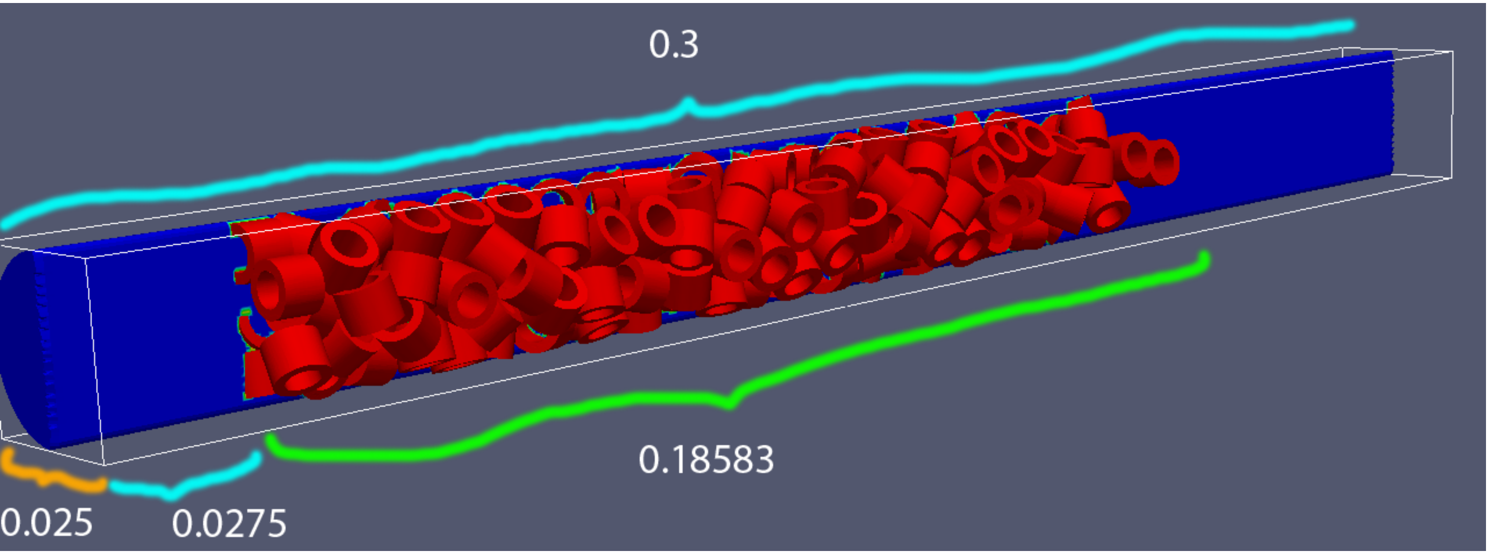
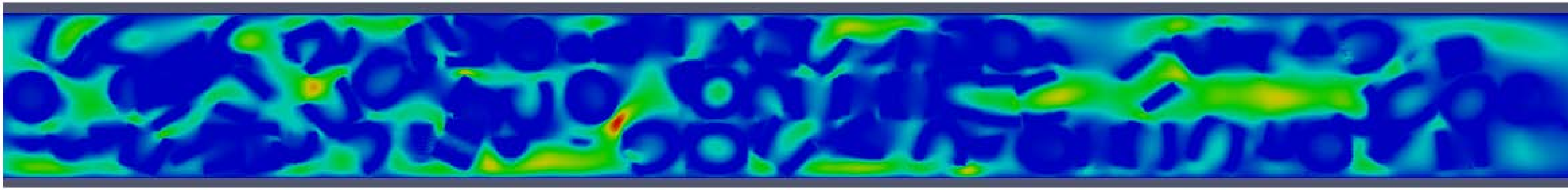
Packed Bed Reactor

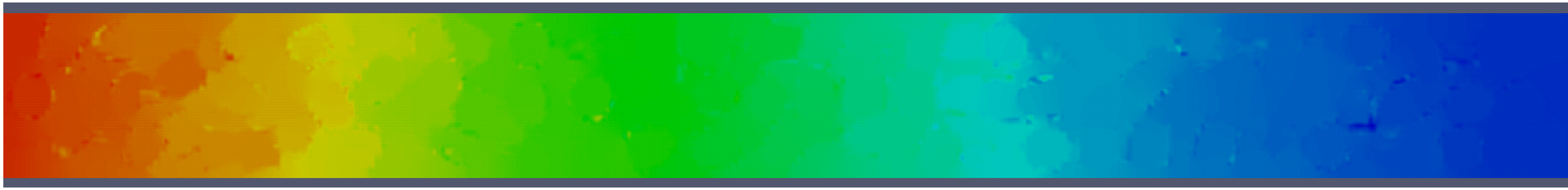


$$v_{mean} = (1 \mid 0.1 \mid 0.01)\, ms^{-1}$$
$$\rho = 1.25\ g\ cm^{-3}$$
$$\mu = 17.57\ 10^{-6}\ Pa\ s$$

Velocity distribution

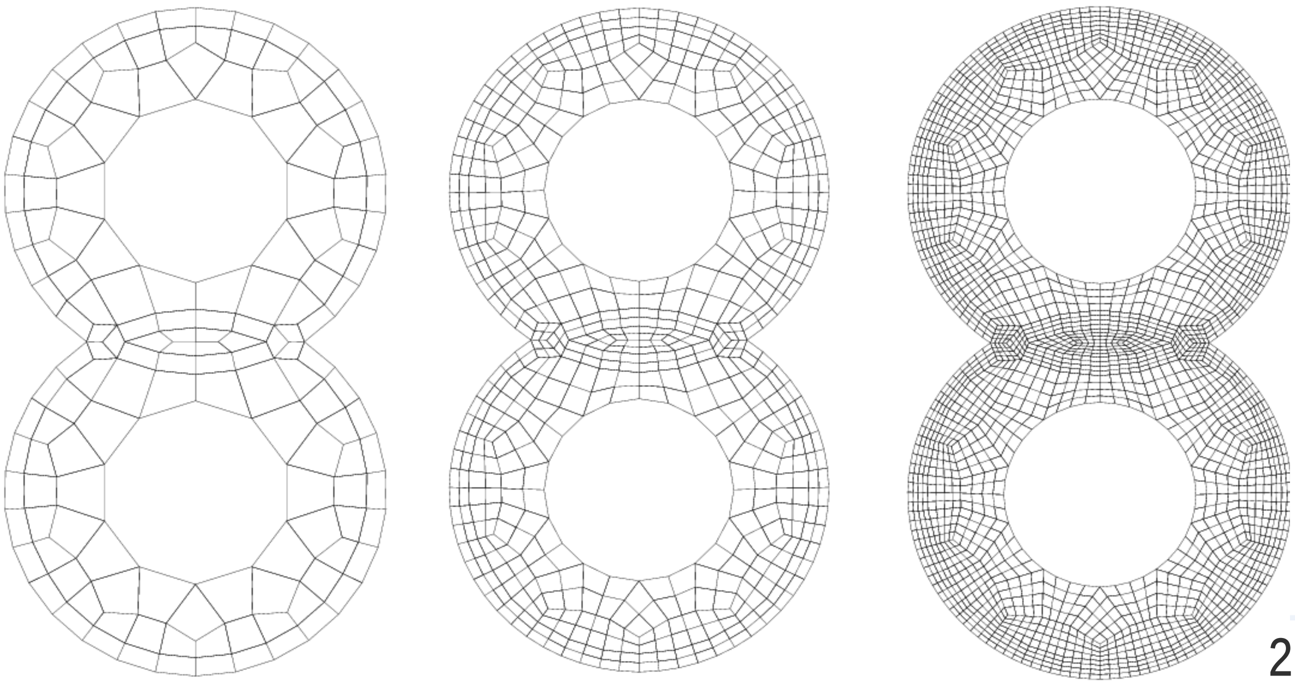


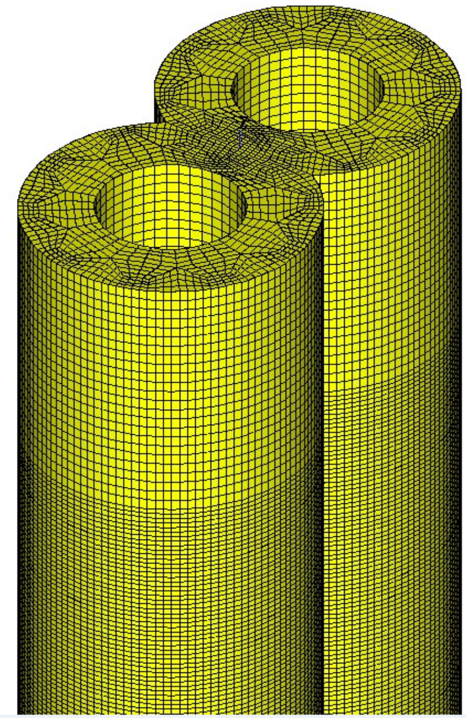
Pressure distribution



Meshing strategy – Hierarchical mesh refinement

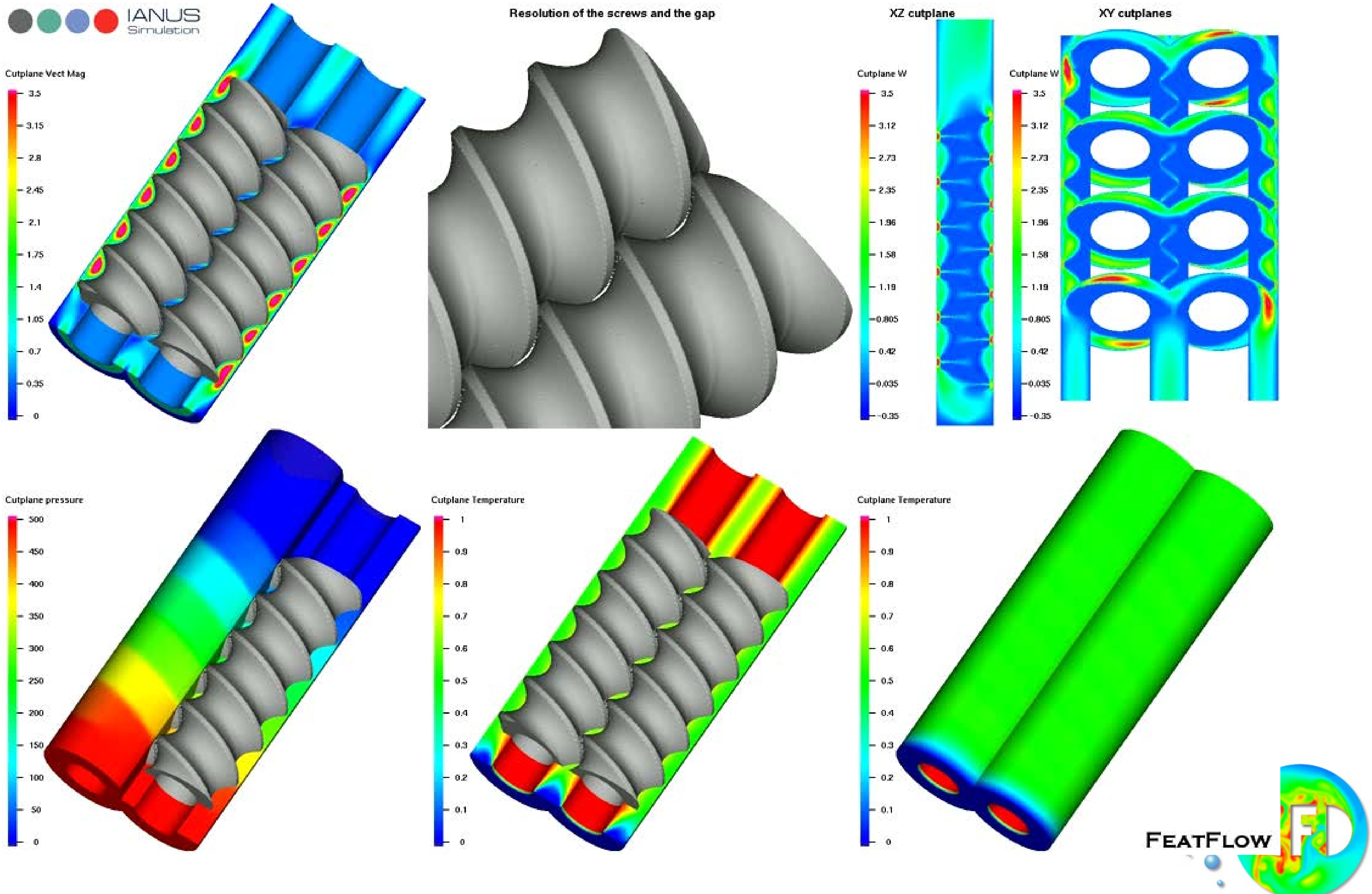
level 1 level 2 level 3





2D mesh extrusion into 3D

Pre-refined regions in the vicinity of gaps.


IANUS
Simulation
Cutplane Vect Mag
3.5 3.15 2.8 2.45 2.1 1.75 1.4 1.05 0.7 0.35 0
Resolution of the screws and the gap
XZ cutplane
Cutplane W
3.5 3.12 2.73 2.35 1.96 1.58 1.19 0.805 0.42 0.035 -0.35
XY cutplanes
Cutplane W
3.5 3.12 2.73 2.35 1.96 1.58 1.19 0.805 0.42 0.035 -0.35
Cutplane pressure
500 450 400 350 300 250 200 150 100 50 0
Cutplane Temperature
1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0
Cutplane Temperature
1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0
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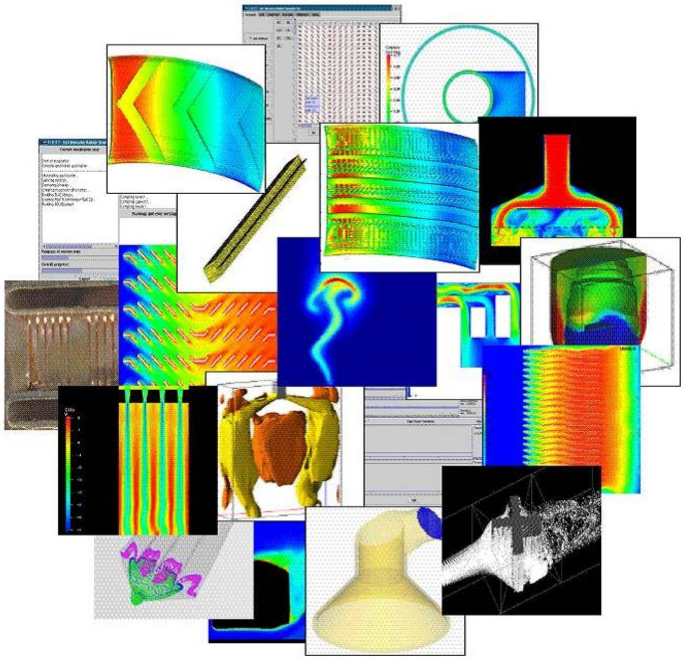
Outlook

- Implementation of a two-equation turbulence model in parallel.
- Parallel implementation of PBEs.
- Reaction coupled dispersed phase flow: liquid-liquid/gas/solid.
- Crystallization processes.
- Two-way coupling: Simulation of Liquid-Liquid/Gas cyclone separators



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Thanks ...

References

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- Lehr F., Millies M. and Mewes D., Bubble size distribution and flow fields in bubble columns, *AIChE Journal*, 48-11, pp.2426-2442 , (2002).