Deciphering hydrodynamics of packed columns

Effects of surface textures on gravity driven liquid flow on inclined plate

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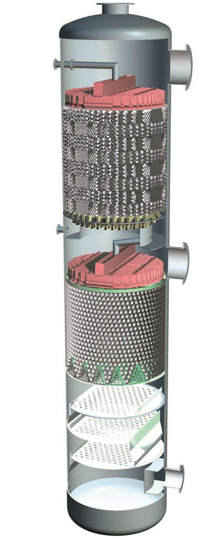
Introduction

Why to pay attention to a flow on a plate

Numerous applications, our concentration lies in deciphering flow in separation columns



[Sulzer ChemTech]

Hydrodynamics

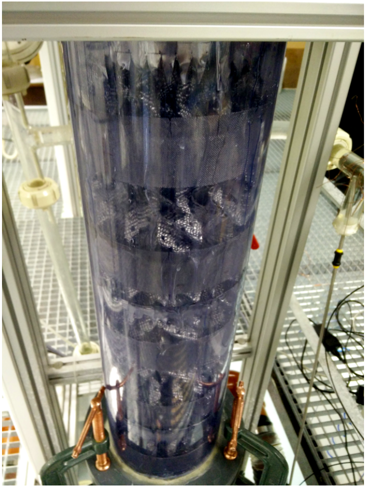
- Fuel cells
  - water management inside PEMFC fuel cells
- Aerospace engineering
  - in flight formation of rivulets on plane wings

Gas-liquid interface

- Packed columns
  - wetting performance
  - mass transfer coefficients
- Catalytic reactors
  - wetting of the catalyst

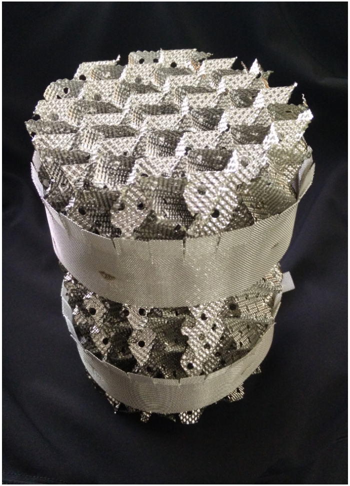
Packed column

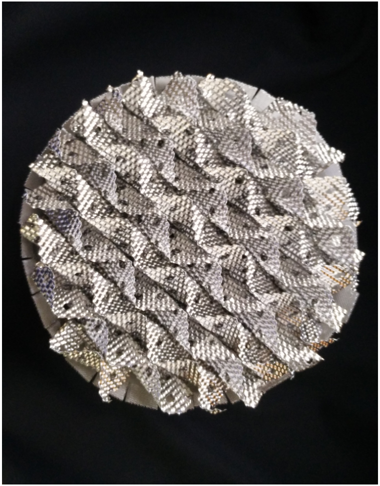
Complex multiphase flow



Structured packing

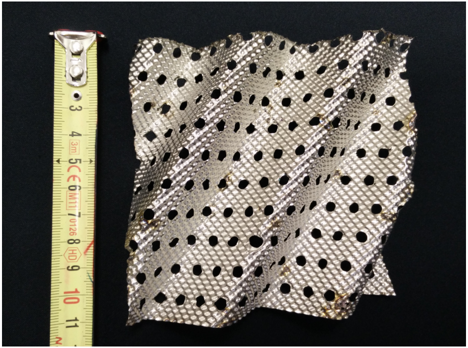
Curled, textured, perforated plate





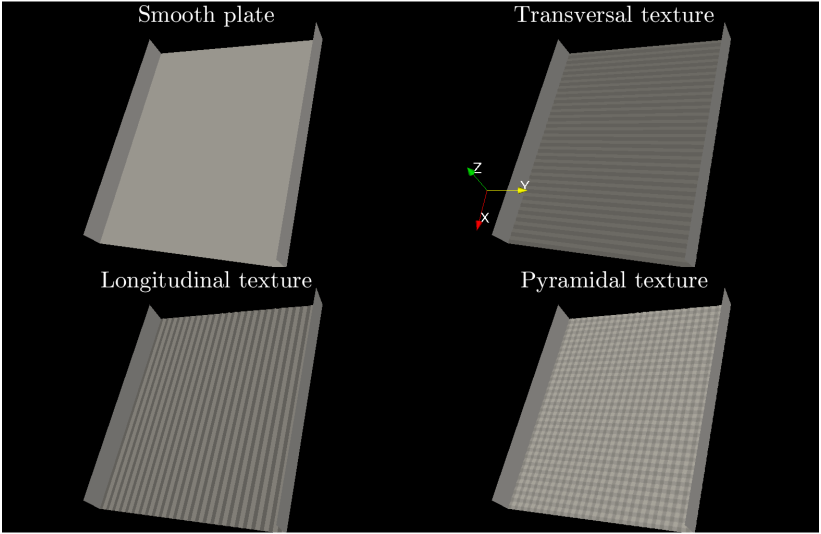
Structured packing – detail

Curled, textured, perforated plate



Structured packing – approximation

First step, flow on an inclined plate equipped with different types of texture



Methodological background

Separation columns modeling

Multiphase hydrodynamics, simultaneous mass and heat transfer, no chemical reaction

Momentum and continuity equations, N phases

$$\rho_i \frac{\partial}{\partial t}(u_i) + \nabla \cdot (\rho_i u_i \otimes u_i + p_i E) = \nabla \cdot \tau + F_i, \quad i = 1, \ldots, N$$

$$\rho_i = \rho(c_i, T_i), \quad \nabla \cdot (u_i) = S_i^{\rho} = \sum_{j=1}^{M} \hat{R}_{i,j}^{c}$$

Mass transfer (no reaction), M species

$$\frac{\partial}{\partial t} c_{i,j} + \nabla \cdot (u_i \, c_{i,j}) = \nabla \cdot \left(\Gamma_{i,j}^{c} \, \nabla c_{i,j}\right) + S_{i,j}^{c}, \qquad j = 1, \ldots, M$$

Heat transfer (no reaction), N phases

$$\frac{\partial}{\partial t} T_i + \nabla \cdot (u_i \, T_i) = \nabla \cdot \left(\Gamma_i^{T} \, \nabla T_i\right) + S_i^{T}, \qquad i = 1, \ldots, N$$

Actually solved equations

Isothermal case, incompressible fluids, flow driven by gravity, no mass transfer

Momentum and continuity equations

$$u_t + \nabla \cdot (u \otimes u) - \nabla \cdot (\mu \nabla u) - (\nabla u) \cdot \nabla \tilde{h} = $$
$$= - \nabla p_d - g \cdot x \otimes \nabla \rho + \gamma \kappa \nabla \tilde{h}$$
$$\nabla \cdot u = 0$$

Advection equation for gas-liquid interface (GLI)

$$\tilde{h}_t + \nabla \cdot (u \tilde{h}) + \nabla \cdot \left[u_r \tilde{h} (1 - \tilde{h}) \right] = 0$$

Notations

$u[\mathrm{m\,s^{-1}}]$ .... bulk velocity

$u_r[\mathrm{m\,s^{-1}}]$ .. compression velocity

$\mu[\mathrm{Pa\,s}]$ .... dynamic viscosity

$\rho[\mathrm{kg\,m^{-3}}]$ .... density

$\gamma[\mathrm{N\,m^{-1}}]$ .... surface tension

$g[\mathrm{m\,s^{-2}}]$ gravitational acceleration

$x[\mathrm{m}]$ ....position vector

$\tilde{h}[-]$ ....GLI tracking function

Reynolds number

$$\mathrm{Re} = \frac{\rho U L}{\mu} = \frac{U L}{\nu}$$

U ... film velocity scale, L ... film characteristic dimension (thickness)
ρ ... liquid density, μ, ν ... liquid dynamic/kinematic viscosity

$$\mathrm{Re} = \frac{\text{inertia}}{\text{viscosity}}$$

Weber number

$$\mathrm{We} = \frac{\rho U^2 L}{\gamma}$$

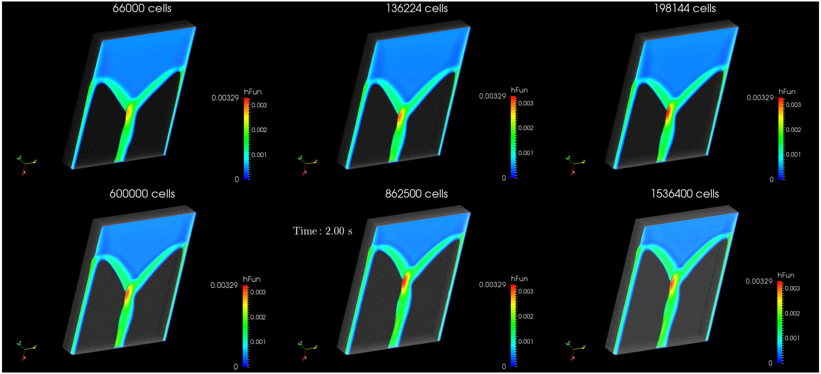
U ... film velocity scale, L ... film characteristic dimension (thickness)
ρ ... liquid density, γ ... gas-liquid surface tension

$$\mathrm{We} = \frac{\text{inertia}}{\text{capillarity}}$$

Discretization schemes

Attempts on optimization of the discretion schemes for the given task

Mesh: $6 \times 5 \times 0.7\,\mathrm{cm}$ geometry, $66000 - 1500000$ hex cells,
$\mathrm{Re}_I = 124,\ \mathrm{We} = 0.71$



Discretization schemes

Attempts on optimization of the discretion schemes for the given task

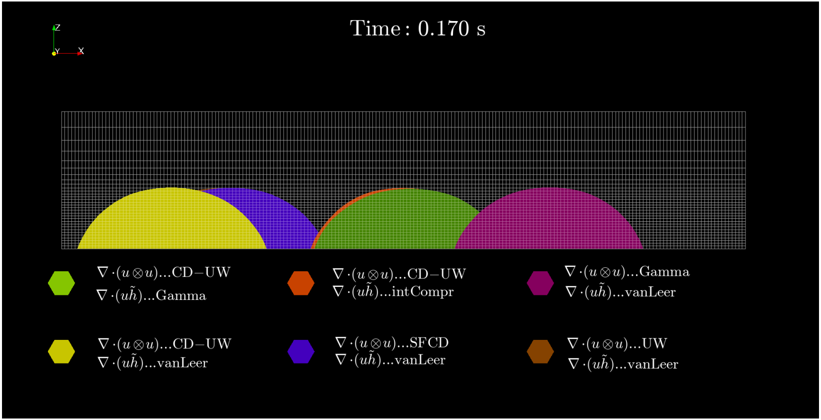
Term	Used scheme
$u_t, \tilde{h}_t$	implicit Euler
$\nabla \cdot (u \otimes u)$	Upwind differencing (UD)
$\nabla \cdot (\mu \nabla u)$	Central differencing (CD)
$\nabla \cdot (u\tilde{h})$	CD-UD with van Leer limiter
$\nabla \cdot \left[u_r \tilde{h}(1-\tilde{h})\right]$	Central differencing (CD)
$\nabla \cdot u$	Central differencing (CD)

Table : Default `ddtSchemes` and `divSchemes`

Commentary

- Generally stable settings but UD is highly diffusive and the choice of van Leer limiter might be questionable
- Problem is highly dependent on surface forces and thus on interface sharpness

Case: Spreading of 2D droplet, $R_0 = 2\,\mathrm{mm}$, $h_0 = 0.7\,\mathrm{mm}$, $\theta_\infty = 70°$



Discretization schemes

Attempts on optimization of the discretion schemes for the given task

Term	Used scheme
$u_t, \tilde{h}_t$	Crank-Nicolson blended with Euler
$\nabla \cdot (u \otimes u)$	Self-filtered central differencing (SFCD)
$\nabla \cdot (\mu \nabla u)$	Central differencing (CD)
$\nabla \cdot (u\tilde{h})$	Gamma with $\beta = 0.25$
$\nabla \cdot \left[u_r \tilde{h}(1 - \tilde{h})\right]$	Interface compression
$\nabla \cdot u$	Central differencing (CD)

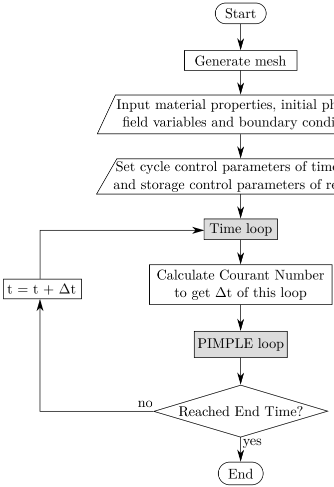
Table : "Optimized" `ddtSchemes` and `divSchemes`

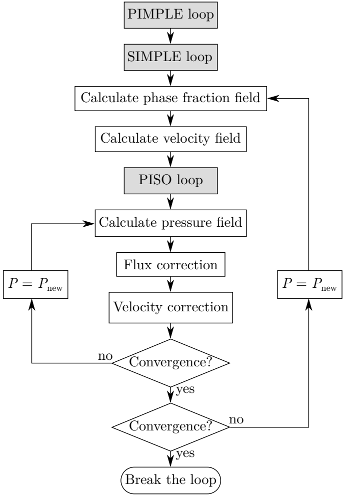
Commentary

- The schemes are modified to make use of physical bounds on the simulated quantities

Simulation scheme

PIMPLE algorithm with adaptive time step

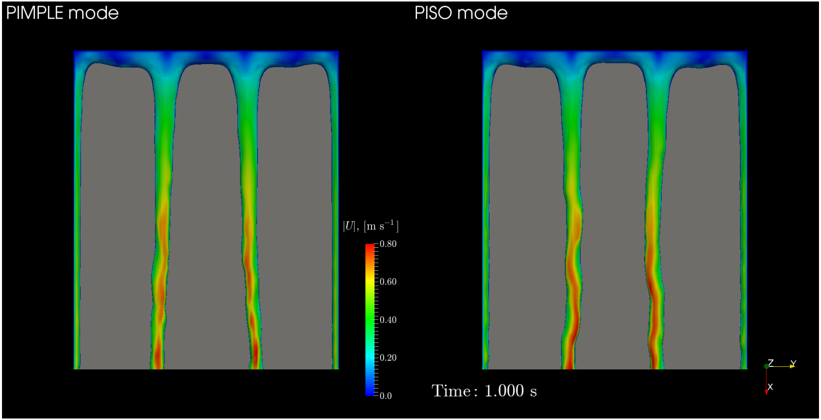




PIMPLE vs. PISO algorithms

PIMPLE: improved stability and control BUT at higher computational cost

Mesh: 0.3 millions of ”hex” cells, graded in z-axis direction
smooth plate, $\mathrm{Re}_I = 62, \ \mathrm{We} = 0.18$



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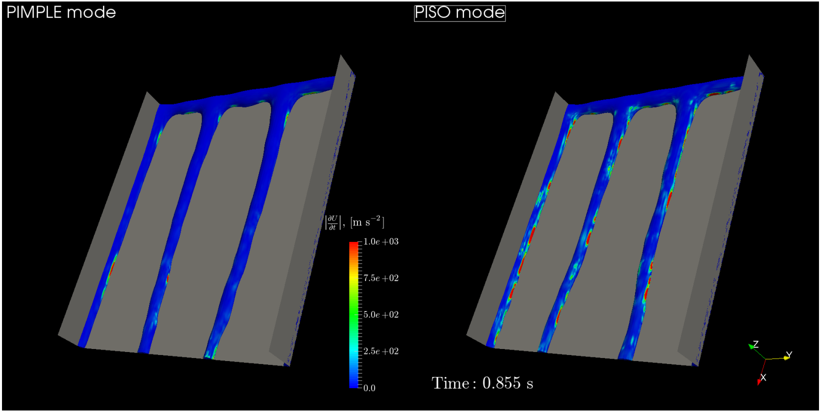


Used methods of numerical linear algebra

Solvers for large (sparse) systems of linear algebraic equations (SLAE)

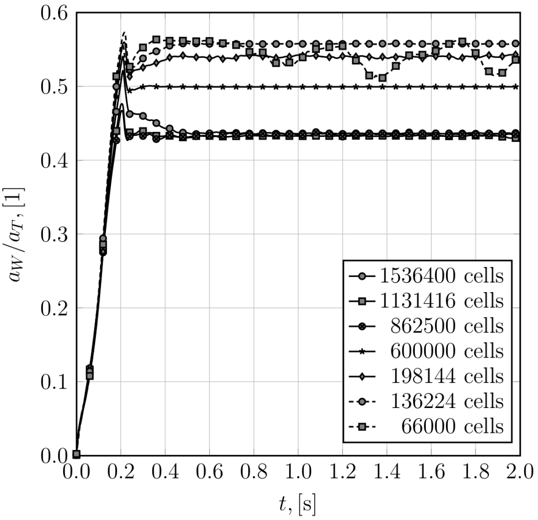
General notes

For the solved class of problems,

- Meshes usually have 1^{+}MM cells $\rightarrow$ systems with millions of unknowns
- Phase volume fraction field behaves "well"
  - No preconditioning nor advanced solvers are needed for solving the resulting SLAE.
  - Gauss-Seidel method is more than enough (usually converges in 1 or 2 iterations).
- Pressure correction equation is a bit more complicated
  - Krylov subspaces based solver, *preconditioned conjugate gradient* (PCG) has to be employed
  - Rather expensive and powerful preconditioner is necessary (used are *fast incomplete Cholesky decomposition* (FDIC) and *geometric multigrid methods* (GAMG).

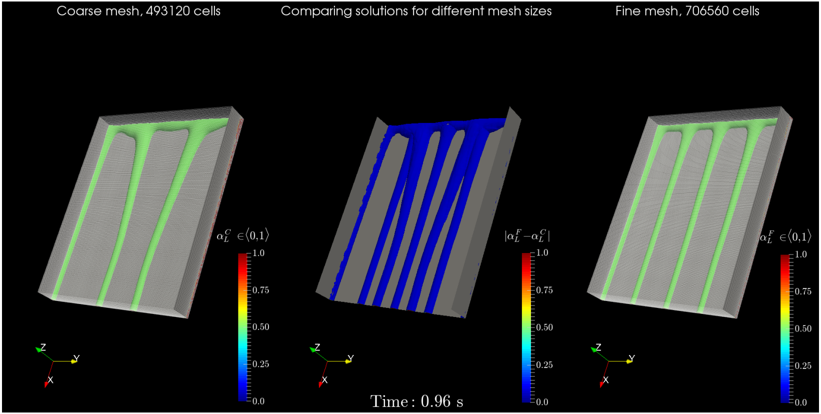
Mesh size optimization idea 1: Follow the variable of interest,

$$\mathrm{Re}_I = 124,\ \mathrm{We} = 0.71$$



Mesh size optimization idea 2: Compare the α_L fields,

$$\mathrm{Re}_I = 62,\ \mathrm{We} = 0.18$$

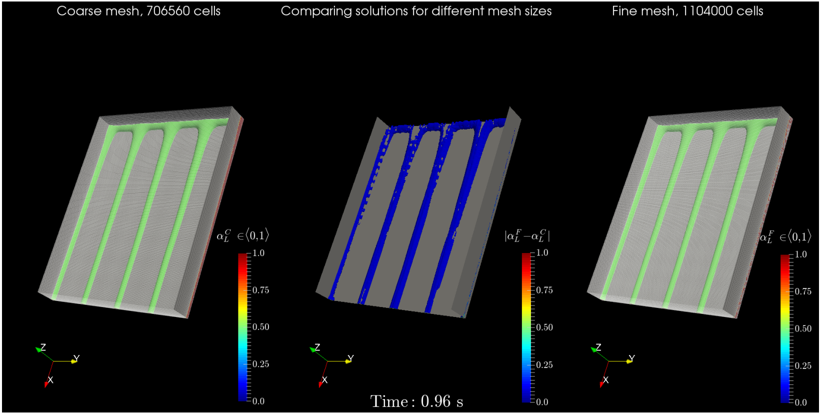


Mesh size optimization mechanisms

Two main approaches to mesh size optimization

Mesh size optimization idea 2: Compare the α_L fields,

$$\mathrm{Re}_I = 62,\ \mathrm{We} = 0.18$$



Mesh size optimization mechanisms

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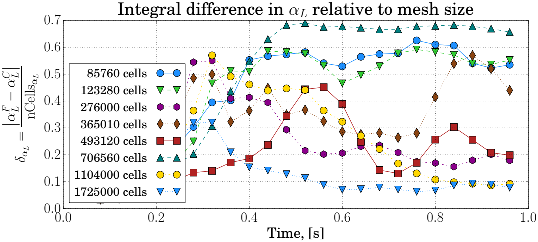
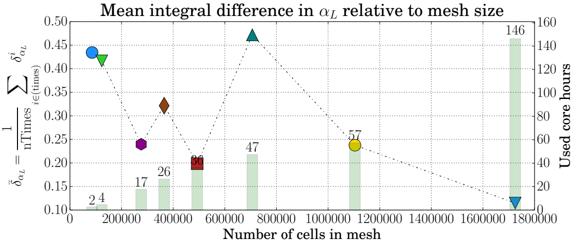
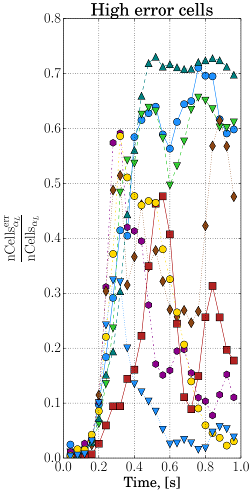




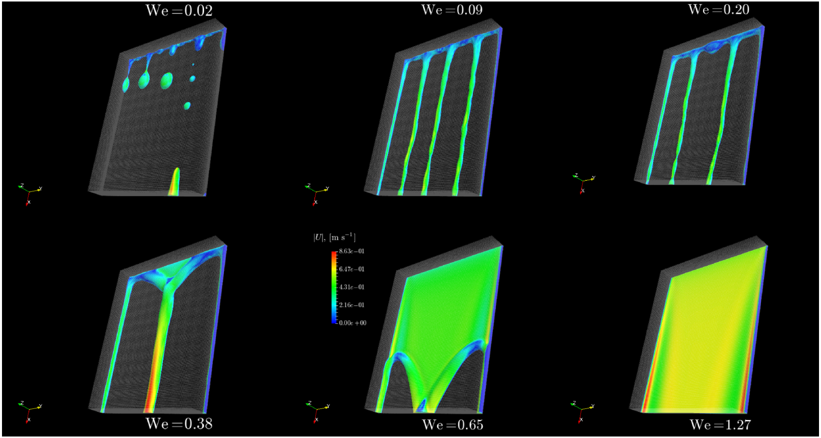


Results

Flow on a smooth plate

blockMesh generated mesh consisting of 1140000 cells

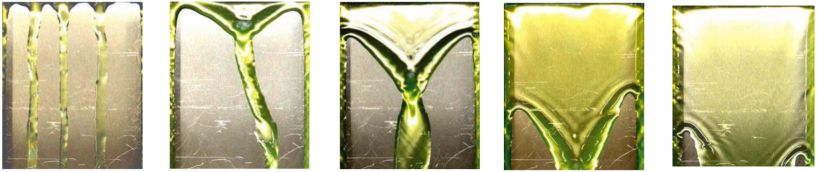
Wetted to total area ratio: Flow regimes in dependence on We



Flow on a smooth plate

blockMesh generated mesh consisting of 1140000 cells

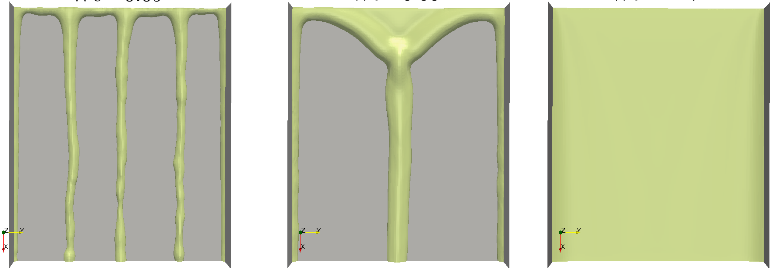
Wetted to total area ratio: Flow regimes in dependence on We



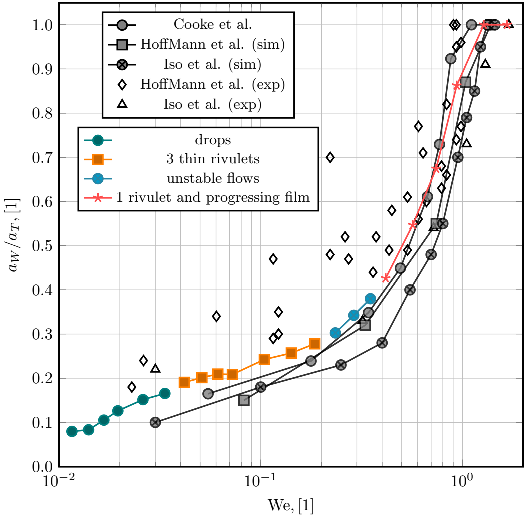
(a) $\mathrm{We}_{l\,\mathrm{N}}$ =0.05 (b) $\mathrm{We}_{l\,\mathrm{N}}$ =0.33 (c) $\mathrm{We}_{l\,\mathrm{N}}$ =0.73 (d) $\mathrm{We}_{l\,\mathrm{N}}$ =1.01 (e) $\mathrm{We}_{l\,\mathrm{N}}$ =1.32

[Yoshiuki I. et al. Numerical and experimental study on liquid film flows on packing elements in absorbers for post-combustion CO_2 capture, *Energy Procedia*, **2013**]

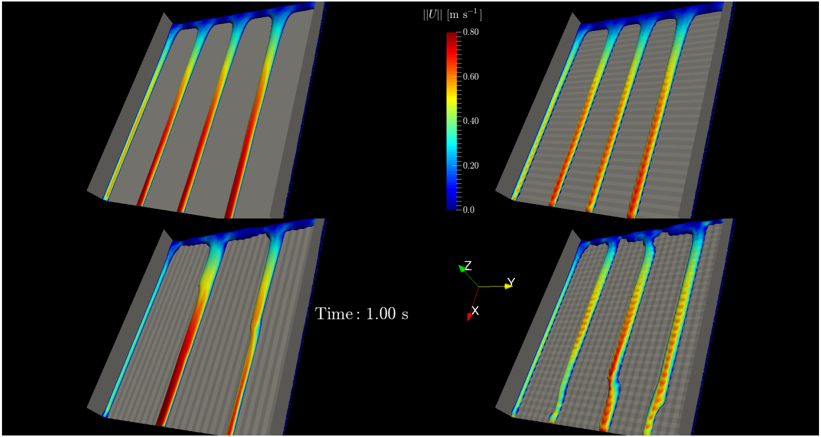
$\mathrm{We} = 0.09$ $\mathrm{We} = 0.38$ $\mathrm{We} = 1.27$



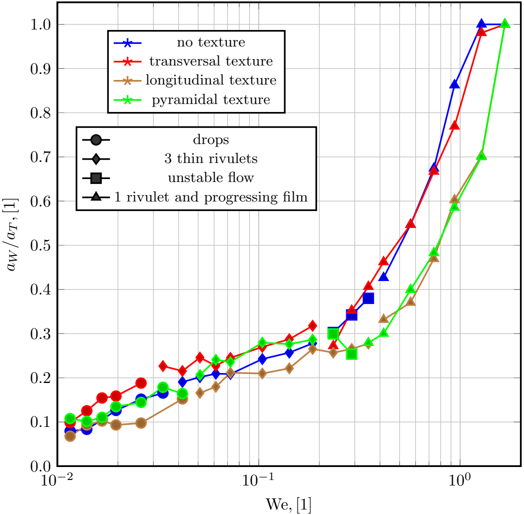
Wetted to total area ratio: Flow regimes in dependence on We



Qualitative comparison: Effects of textures



Quantitative comparison: Wetted to total area ratio



Conclusion

Concluding remarks

Development of the simulations somehow mimicking the flow in packed columns

Flow on a smooth plate

- Already available:
  - Simulation results in agreement with the published data
  - Identification of flow regimes in dependence on Re, We New
- Outlook:
  - Study of the influence of boundary conditions on the solution
  - Study of wetting in dependence on plate inclination and liquid type

Flow on a textured plate

- Already available:
  - Automatic geometry creation and meshing (transversal, longitudinal and pyramidal texture New)
- Outlook:
  - Texture optimization (density, roughness) $\Longleftrightarrow$ Reduced Order Modeling
  - Include snappyHexMesh in the mesh creation process

Acknowledgments

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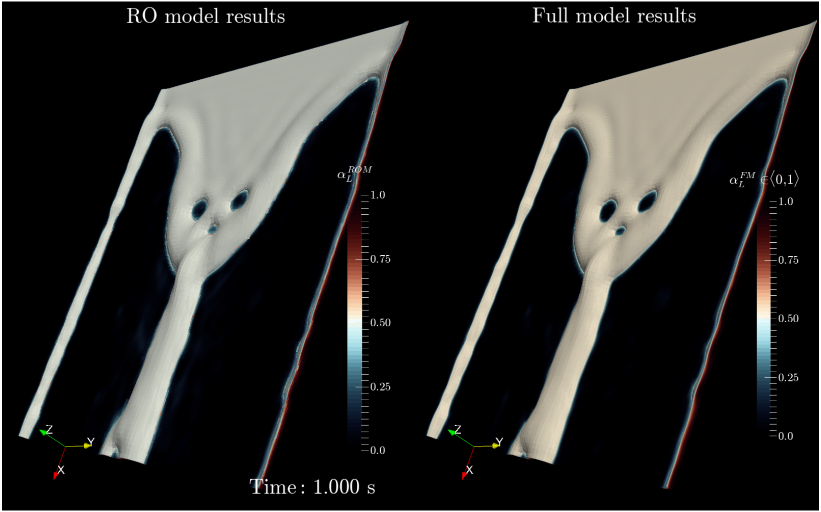
[8] ——, "Detailed investigation of multiphase (gas-liquid and gas-liquid-liquid) flow behaviour on inclined plates." *Chemical Engineering Research and Design*, vol. 84, no. A2, pp. 147–154, 2006.

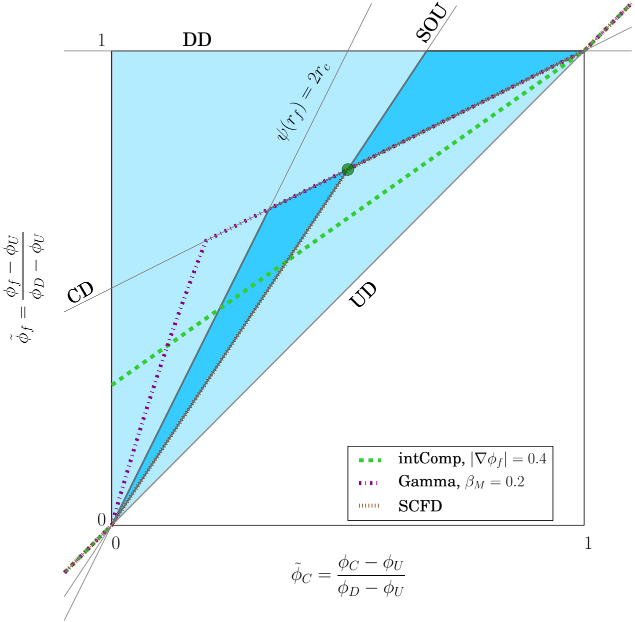
Thank you for your attention

Qualitative comparison: Reduced order vs. full model



Convective terms discretization

NVD of the used convective terms



Simulation control

Altix UV 2000, 1.1MM of hex cells, 4 cores