

Deciphering hydrodynamics of packed columns

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



Martin Isoz

UCT Prague,
Department of mathematics



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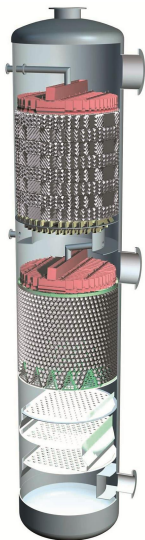


Introduction



Why to pay attention to a flow on a plate

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



[Sulzer ChemTech]

Hydrodynamics

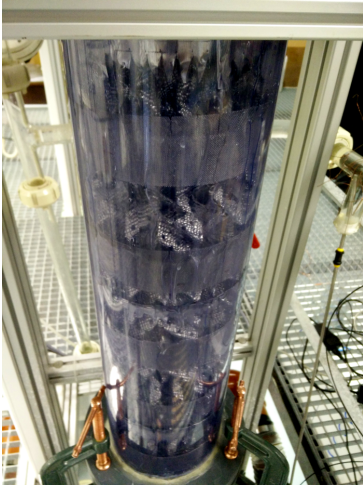
- Fuel cells
 - water management inside PEMFC fuel cells
- Aerospace engineering
 - in flight formation of rivulets on plane wings

Gas-liquid interface

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

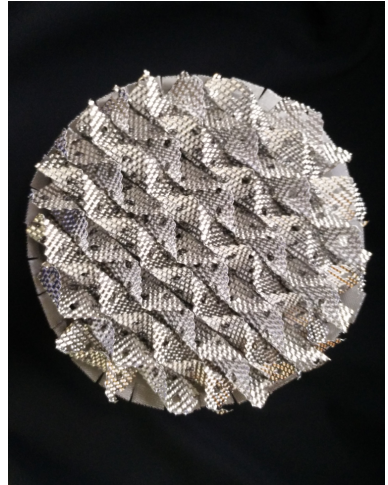
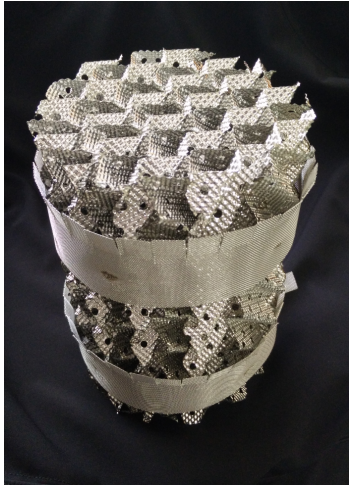
Packed column

Complex multiphase flow



Structured packing

Curled, textured, perforated plate



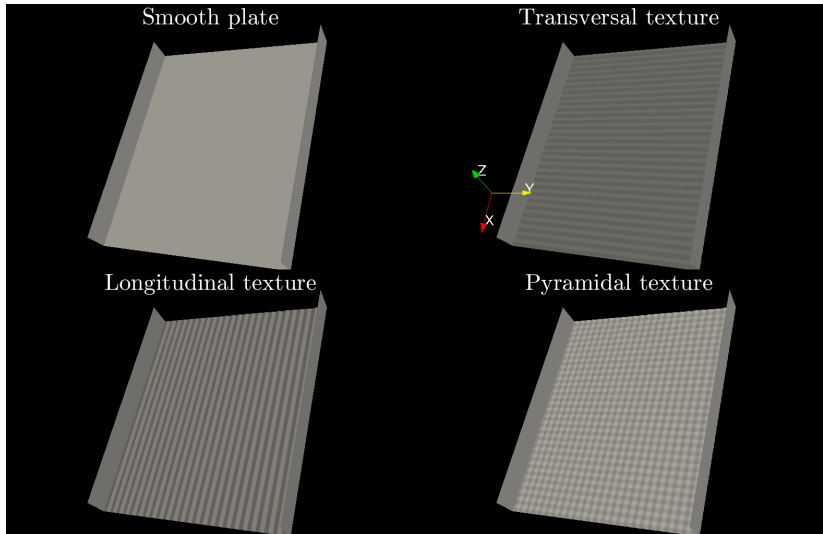
Structured packing – detail

Curled, textured, perforated plate



Structured packing – approximation

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





Methodological background





Momentum and continuity equations, N phases

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

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

Mass transfer (no reaction), M species

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

Heat transfer (no reaction), N phases

$$\frac{\partial}{\partial t} T_i + \nabla \cdot (u_i T_i) = \nabla \cdot (\Gamma_i^T \nabla T_i) + S_i^T, \quad i = 1, \dots, N$$

Actually solved equations

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



Momentum and continuity equations

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

Advection equation for gas-liquid interface (GLI)

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

Notations

$u[\text{m s}^{-1}]$	bulk velocity	$\gamma[\text{N m}^{-1}]$	surface tension
$u_r[\text{m s}^{-1}]$..	compression velocity	$g[\text{m s}^{-2}]$	gravitational acceleration
$\mu[\text{Pa s}]$	dynamic viscosity	$x[\text{m}]$	position vector
$\rho[\text{kg m}^{-3}]$	density	$\tilde{h}[-]$	GLI tracking function



Reynolds number

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

U ... film velocity scale, L ... film characteristic dimension (thickness)

ρ ... liquid density, μ, ν ... liquid dynamic/kinematic viscosity

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

Weber number

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

U ... film velocity scale, L ... film characteristic dimension (thickness)

ρ ... liquid density, γ ... gas-liquid surface tension

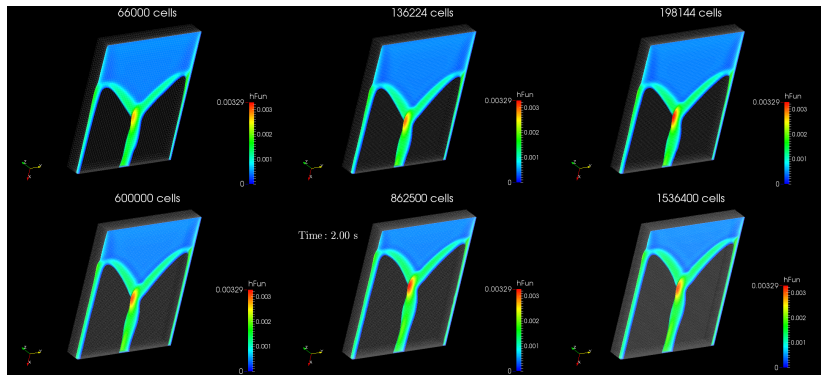
$$\text{We} = \frac{\text{inertia}}{\text{capillarity}}$$

Discretization schemes

Attempts on optimization of the discretion schemes for the given task



Mesh: $6 \times 5 \times 0.7$ cm geometry, 66000 – 1500000 hex cells,
 $Re_I = 124$, $We = 0.71$





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
$\nabla \cdot [u_r \tilde{h}(1 - \tilde{h})]$	
$\nabla \cdot u$	Central differencing (CD)

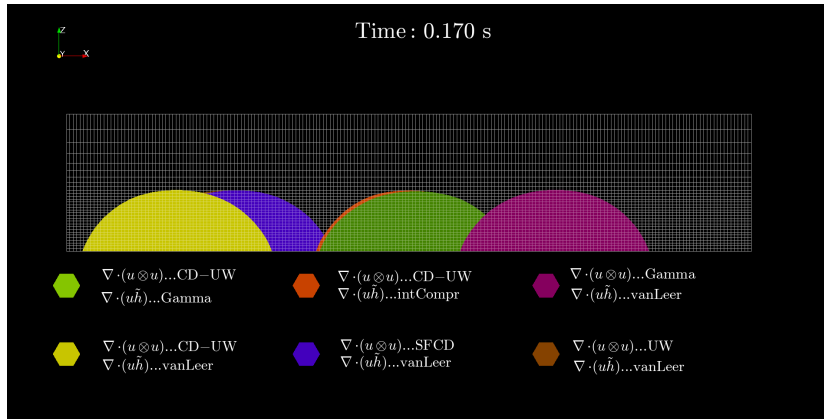
Table : Default `ddtSchemes` and `divSchemes`

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, $R_0 = 2$ mm, $h_0 = 0.7$ mm, $\theta_\infty = 70^\circ$





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 $\beta = 0.25$
$\nabla \cdot [u_r \tilde{h}(1 - \tilde{h})]$	Interface compression
$\nabla \cdot u$	Central differencing (CD)

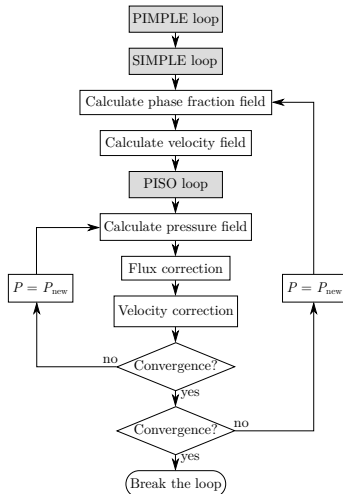
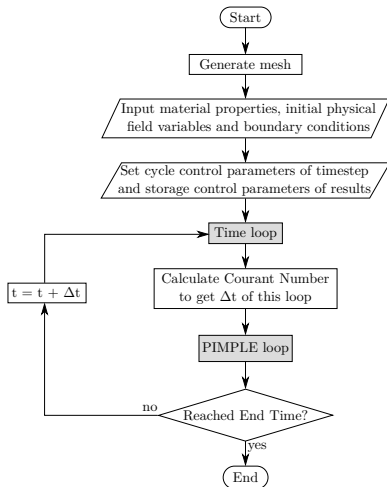
Table : "Optimized" ddtSchemes and divSchemes

Commentary

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

Simulation scheme

PIMPLE algorithm with adaptive time step

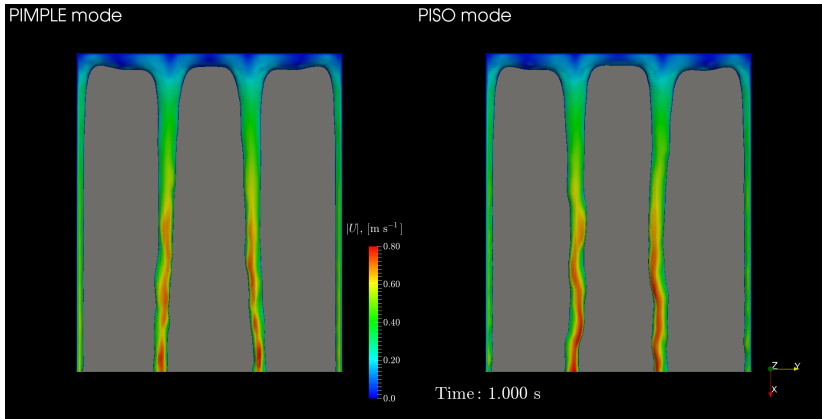


PIMPLE vs. PISO algorithms

PIMPLE: improved stability and control BUT at higher computational cost



Mesh: 0.3 millions of "hex" cells, graded in z -axis direction
smooth plate, $Re_I = 62$, $We = 0.18$

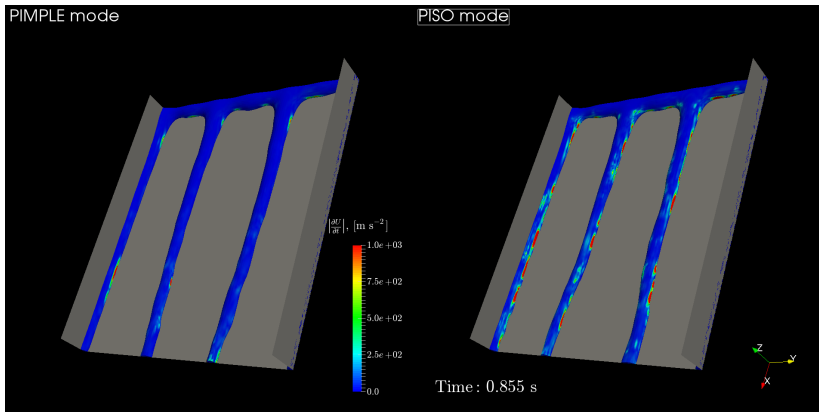


PIMPLE vs. PISO algorithms

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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)).

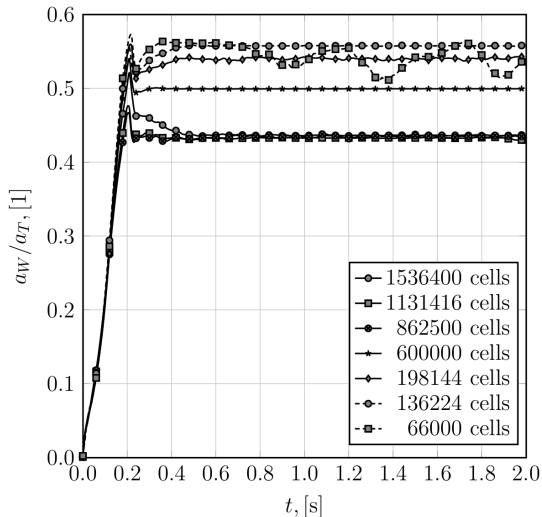
Mesh size optimization mechanisms

Two main approaches to mesh size optimization



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

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

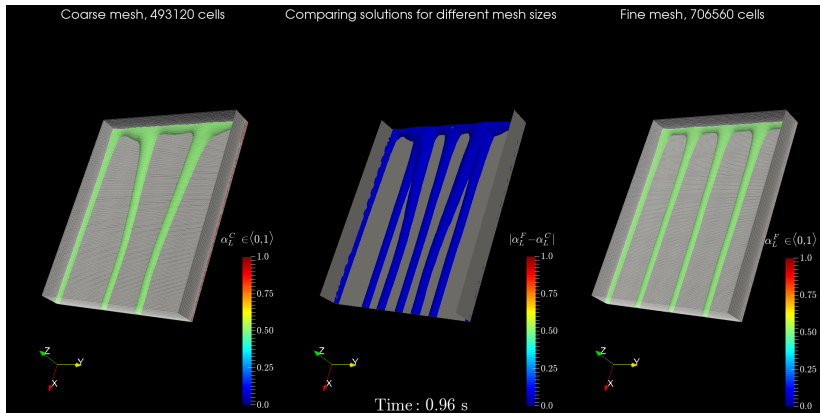


Mesh size optimization mechanisms

Two main approaches to mesh size optimization



Mesh size optimization idea 2: Compare the α_L fields,
 $Re_I = 62$, $We = 0.18$

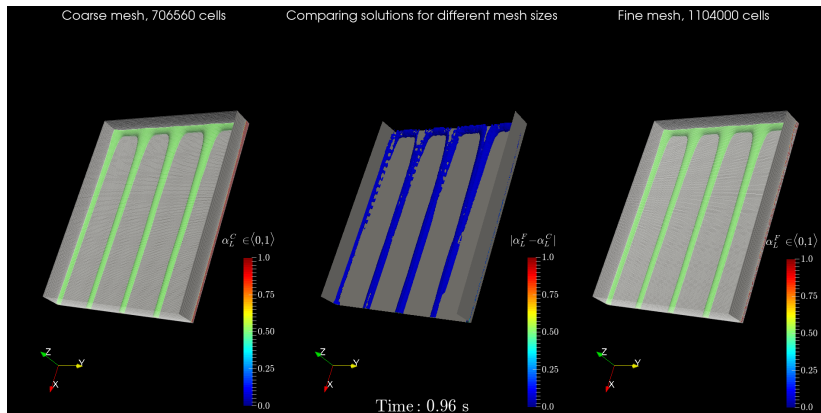


Mesh size optimization mechanisms

Two main approaches to mesh size optimization



Mesh size optimization idea 2: Compare the α_L fields,
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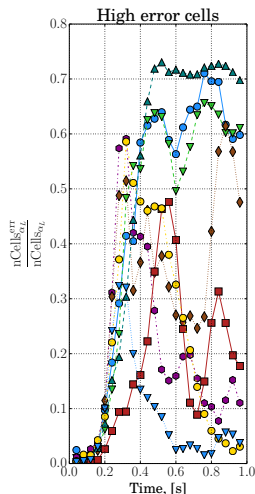
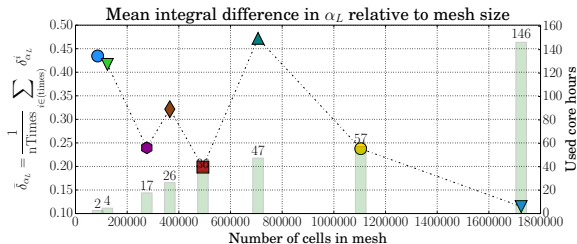
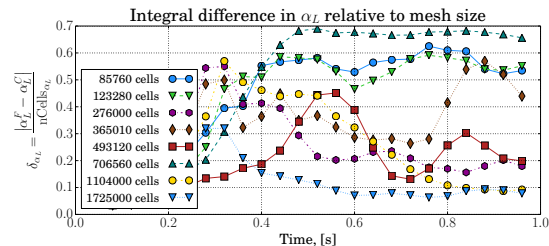


Mesh size optimization mechanisms

Two main approaches to mesh size optimization



Mesh size optimization idea 2: Compare the α_L fields, $Re_I = 62$, $We = 0.18$





Results

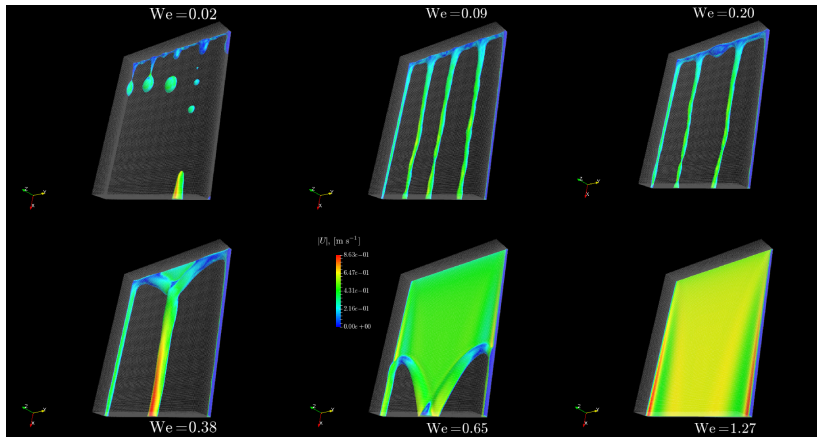


Flow on a smooth plate

blockMesh generated mesh consisting of 1140000 cells



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

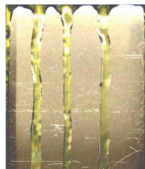


Flow on a smooth plate

blockMesh generated mesh consisting of 1140000 cells



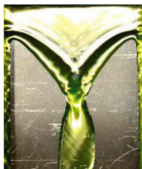
Wetted to total area ratio: Flow regimes in dependence on We



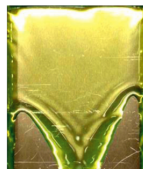
(a) $We_{lN} = 0.05$



(b) $We_{lN} = 0.33$



(c) $We_{lN} = 0.73$



(d) $We_{lN} = 1.01$



(e) $We_{lN} = 1.32$

[Yoshiuki I. et al. Numerical and experimental study on liquid film flows on packing elements in absorbers for post-combustion CO₂ capture, *Energy Procedia*, **2013**]

$We = 0.09$



$We = 0.38$

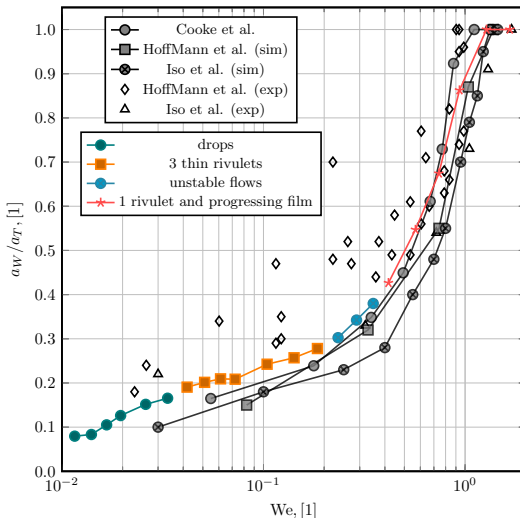


$We = 1.27$

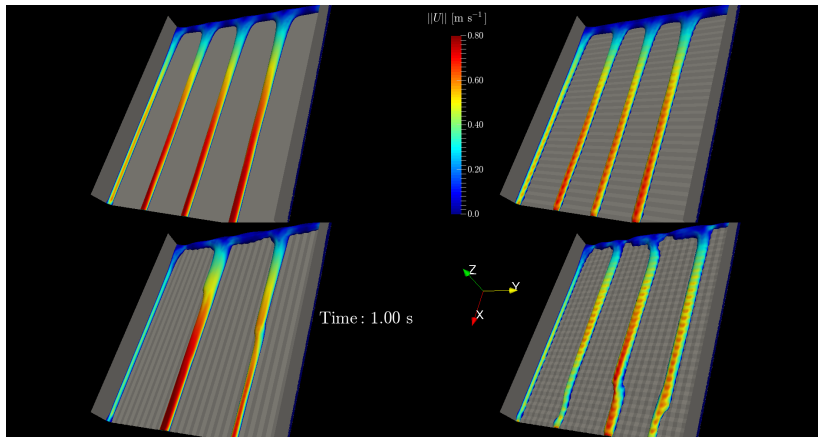




Wetted to total area ratio: Flow regimes in dependence on We

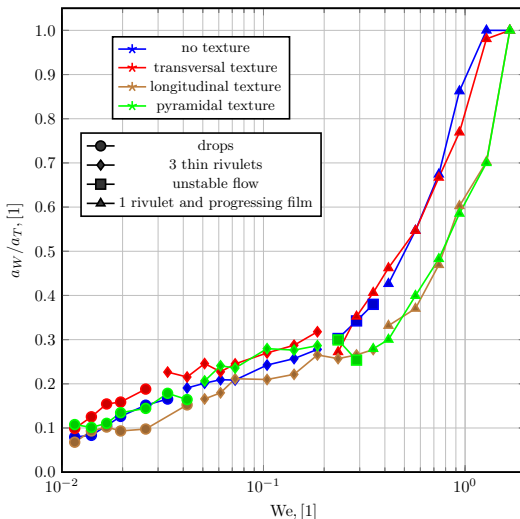


Qualitative comparison: Effects of textures





Quantitative comparison: Wetted to total area ratio





Conclusion





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)
↔ **Reduced Order Modeling**
 - Include snappyHexMesh in the mesh creation process



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- [3] J. J. Cooke, S. Gu, L. M. Armstrong, and K. H. Luo, “Gas-liquid flow on smooth and textured inclined planes.” *World Academy of Science, Engineering and Technology*, vol. 68, pp. 1712–1719, 2012.
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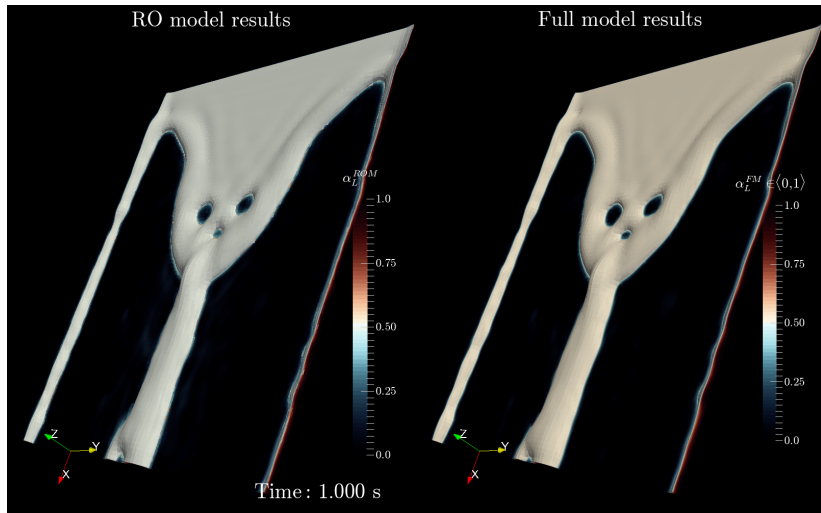
- [6] Y. Haroun, L. Raynal, and P. Alix, “Prediction of effective area and liquid hold-up in structured packings by CFD.” *Chemical Engineering Research and Design*, vol. 92, pp. 2247–2254, 2014.
- [7] A. Hoffmann, I. Ausner, J.-U. Repke, and G. Wozny, “Fluid dynamics in multiphase distillation processes in packed towers.” *Computers & Chemical Engineering*, vol. 29, no. 6, pp. 1433–1437, 2005.
- [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

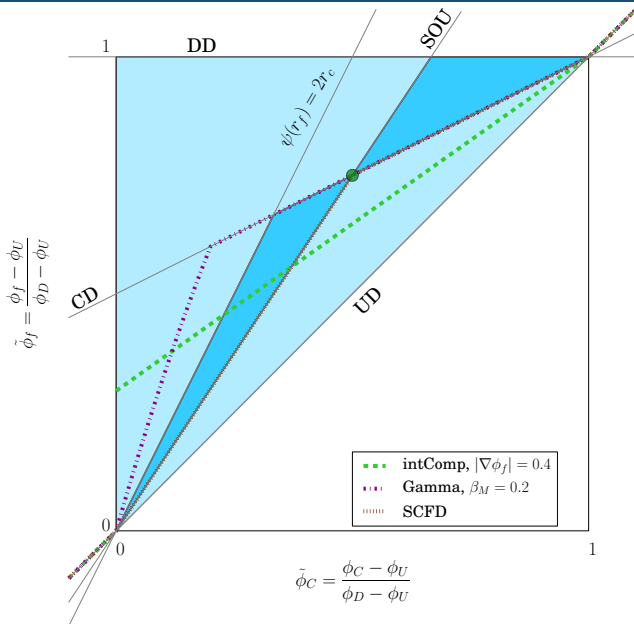


Qualitative comparison: Reduced order vs. full model



Convective terms discretization

NVD of the used convective terms



Simulation control

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



Altix UV 2000, 4 cores, 1.1MM cells, case: iF_Re60.0_60.0_H2OCK_SMV3_INIT,
solver: interFoam -parallel, version: 2.4.0-dcea1e13ff76

