VOF study of gas-liquid multiphase flow in structured separation columns packing

M. Isoz[a]

[a] Institute of Thermomechanics, Academy of Sciences of the Czech Republic

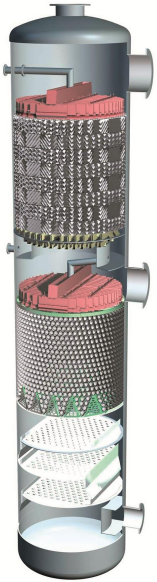
June 17, 2017

12th OpenFOAM Workshop 2017

Introduction

Research motivation

Provide usable tools for separation columns modeling



[Sulzer ChemTech]

Importance

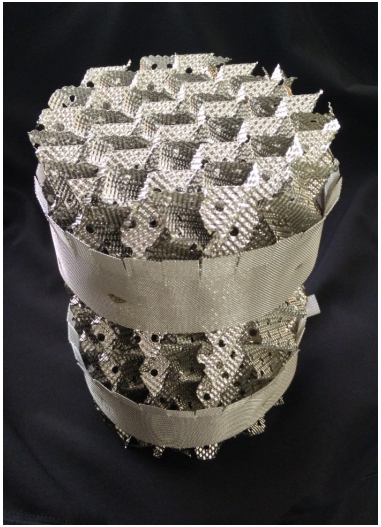
- Chemical industry creates mixtures but sells "pure species" (e.g. oil)
- 2014, 3% of energy consumption of the USA was due to the separation columns

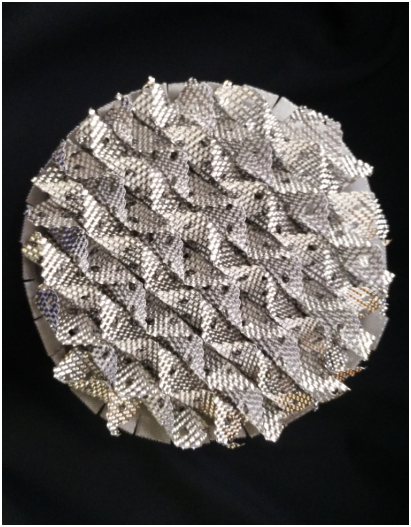
Challenges

- Multiphase flow $\rightsquigarrow$ non-steady process
- Complex geometry
- Simultaneous heat and mass transfer

Mellapak type structured packing

Corrugated, perforated sheet of steel equipped with texture





Separation columns modeling

Multiphase flow, simultanous heat and mass transfer

Mass and momentum balance, N phases

$$\rho_i \frac{\partial}{\partial t}(\mathbf{U}_i) + \nabla \cdot (\rho_i \mathbf{U}_i \otimes \mathbf{U}_i) = \nabla \cdot \mathbb{T} + F_i, \quad i = 1, \ldots, N$$

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

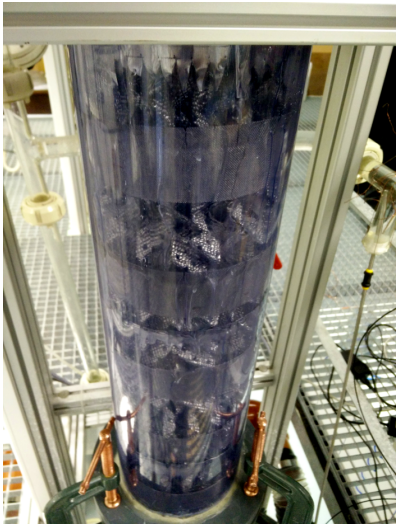
Mass transfer, M species

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

Heat transfer, N phases

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

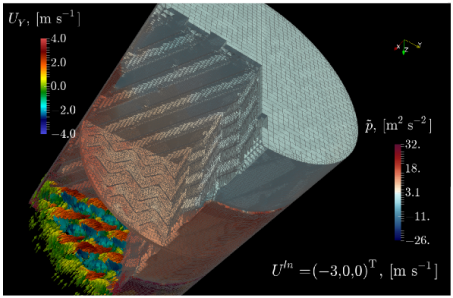
Packed column
Complex multiphase flow

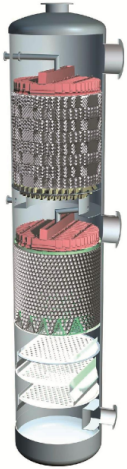


Possible simplifications I

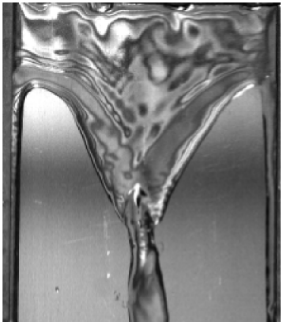
Approach the problem from two different sides

keep geometry,
simplify flow





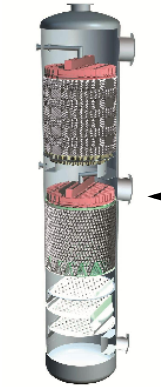
simplify geometry,
keep flow



Possible simplifications II

Simulate different scales and share informations

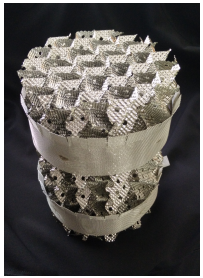
Macro scale



Column

[Sulzer Chemtech]

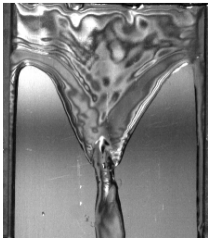
Meso scale



Structured packing

[Sulzer Chemtech]

Micro scale



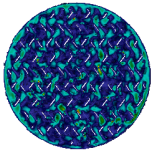
Inclined plate

[Hoffman 2007)]

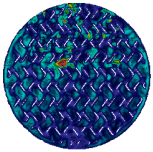
Project goal

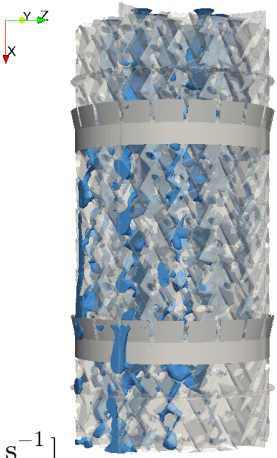
Construct meso scale CFD model of liquid flow in Mellapak type packing

Top $y-z$ slice



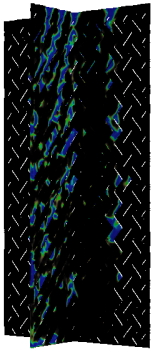
Bottom $y-z$ slice



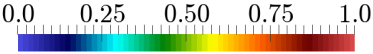


$t = 1.440$ [s]

$x-y$ and $x-z$ slices



$||U||$ [m s^{-1}]



α_L [$-$]

Used models

Single phase steady-state incompressible flows

RANS + SST $k-\omega \rightsquigarrow$ simpleFoam

Navier-Stokes equations

$$\begin{aligned} \mathbf{U}_t + \nabla\cdot(\mathbf{U}\otimes\mathbf{U}) - \nabla\cdot\mathbb{T} &= -\nabla\tilde{p} + \tilde{f} \\ \nabla\cdot\mathbf{U} &= 0 \end{aligned}$$

SST $k-\omega$ model

$$k_t + \mathbf{U}\cdot\nabla k = \tilde{P}_k + \nabla\cdot\left[\left(\nu+\nu_t\sigma_k\right)\nabla k\right] - \beta^* k\omega$$

$$\omega_t + \mathbf{U}\cdot\nabla\omega = \tilde{P}_\omega + \nabla\cdot\left[\left(\nu+\nu_t\sigma_{\omega,1}\right)\nabla\omega\right]\ldots$$

$$\ldots + \alpha S^2 - \beta\omega^2 + 2(1-F_1)\sigma_{\omega,2}\frac{1}{\omega}\nabla k\cdot\nabla\omega$$

BC

$$\begin{aligned} \mathbf{U} &= G(\mathbf{U}) \\ \tilde{p} &= H(p) \\ k &= K(k) \\ \omega &= L(\omega) \\ &\text{on} \quad \partial\Omega^h \end{aligned}$$

IG

$$\mathbf{U}_0, \tilde{p}_0, k_0, \omega_0, \nu_0$$

in Ω^h

Two-phase transient incompressible flows

Immiscible newtonian fluids & VOF modeling ⇝ interFoam

Momentum and continuity equations

$$\partial_t (\rho \mathbf{U}) + \nabla \cdot (\rho \mathbf{U} \otimes \mathbf{U}) - \nabla \cdot (\mu \nabla \mathbf{U}) = -\nabla p_d - \mathbf{g} \cdot \mathbf{h} \nabla \rho + \mathbf{F}_s$$

$$\nabla \cdot \mathbf{U} = 0\,,$$

Advection equation for tracked phase volume fraction

$$\partial_t \alpha + \nabla \cdot (\mathbf{U}\alpha) + \nabla \cdot (\mathbf{U}_r \alpha (1-\alpha)) = 0\,,$$

Notations

$\mathbf{U}[\mathrm{m\,s^{-1}}]$	bulk velocity	$\gamma[\mathrm{N\,m^{-1}}]$	surface tension
$\mathbf{U}_r[\mathrm{m\,s^{-1}}]$	compression velocity	$\mathbf{g}[\mathrm{m\,s^{-2}}]$	gravitational acceleration
$\mu[\mathrm{Pa\,s}]$	dynamic viscosity	$\mathbf{h}[\mathrm{m}]$	reference position vector
$\rho[\mathrm{kg\,m^{-3}}]$	density	$\alpha[-]$	tracked phase volume fraction

Two-phase transient incompressible flows

Immiscible newtonian fluids & VOF modeling ⇝ interFoam

Averaged fluid properties

$$\begin{aligned} \rho &= \alpha\rho_A + (1-\alpha)\rho_B \\ \mu &= \alpha\mu_A + (1-\alpha)\mu_B \end{aligned} \quad , \quad \alpha = \begin{cases} 1, & \text{cell contains only phase } A \\ 0, & \text{cell contains only phase } B \\ a \in (0,1) & \text{cell contains gas-liquid interface}\,. \end{cases}$$

Modeling of the surface forces

$$\mathbf{F}_s = \gamma\,\mathbf{n}\cdot\kappa(\mathbf{x})\,, \quad \mathbf{n} = \frac{\nabla\alpha}{||\nabla\alpha||}\,, \quad \kappa(x) = \nabla\cdot\mathbf{n}\,.$$

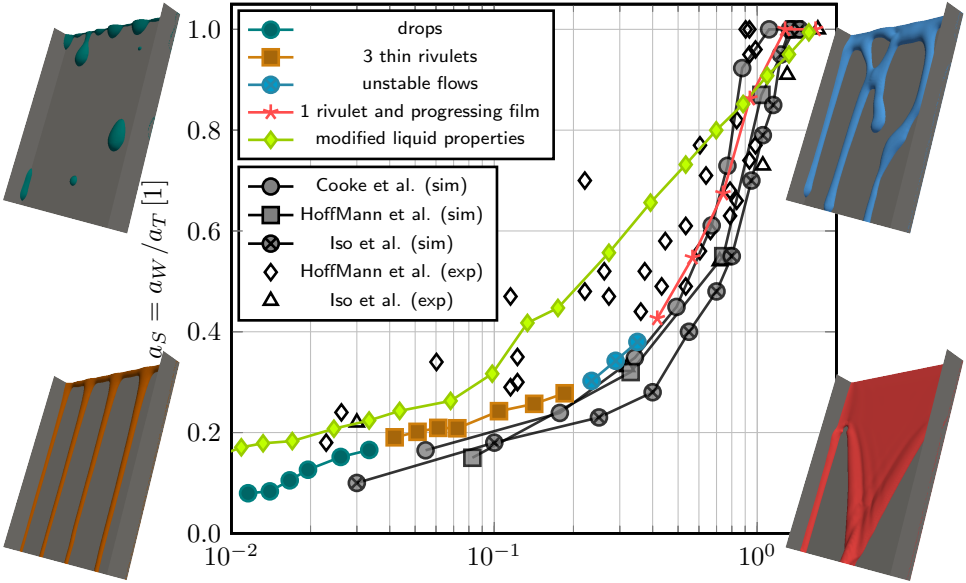
Dynamic contact angle model

$$\mathbf{n}_{wall} = \mathbf{n}_w\cos\theta + \mathbf{t}_w\sin\theta\,, \quad \theta = \theta_0 + (\theta_A - \theta_R)\tanh\left(\frac{u_w}{u_\theta}\right).$$

Preparatory steps

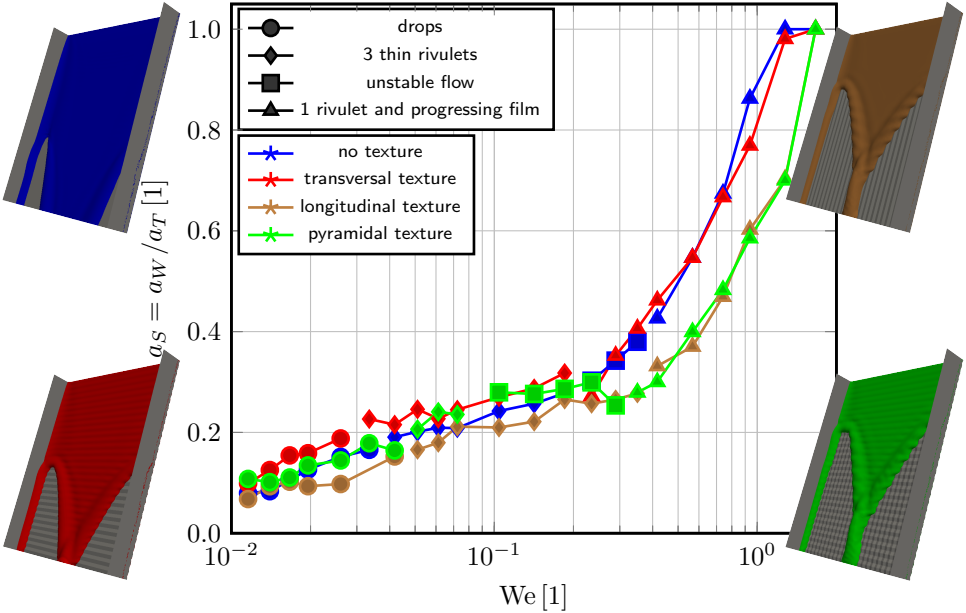
Validation of wetting

Microscale simulations of wetting of inclined plate



Validation of wetting

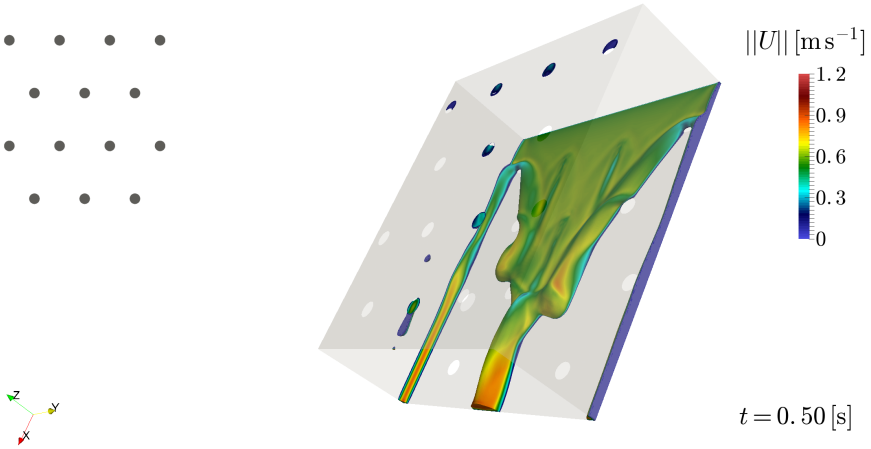
Microscale simulations of wetting of inclined plate



Test of perforation

Modeling of flow between two perforated plates

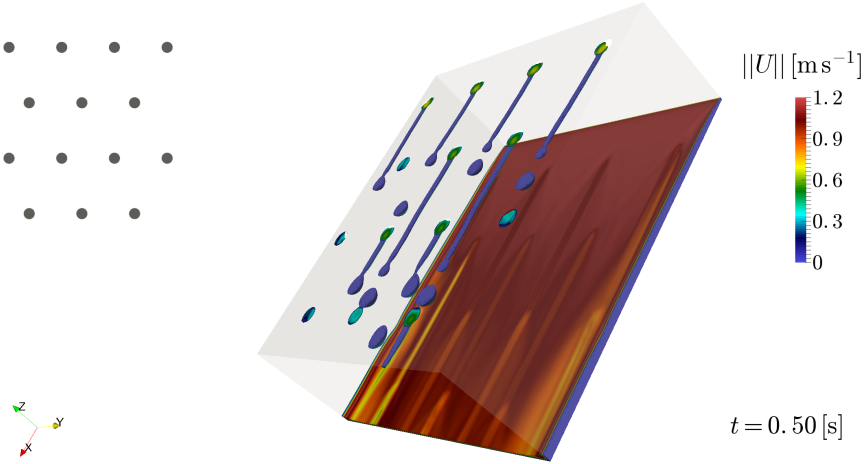
Example: $B = Q_L/\mathrm{Area}(\text{Geometry crossection}) = 40\,[\mathrm{m\,h^{-1}}]$, $d_{\mathrm{perf}} = 3\,[\mathrm{mm}]$



Test of perforation

Modeling of flow between two perforated plates

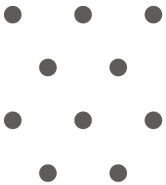
Example: $B = 80\,[\mathrm{m\,h^{-1}}]$, $d_{\mathrm{perf}} = 3\,[\mathrm{mm}]$, different hole positions

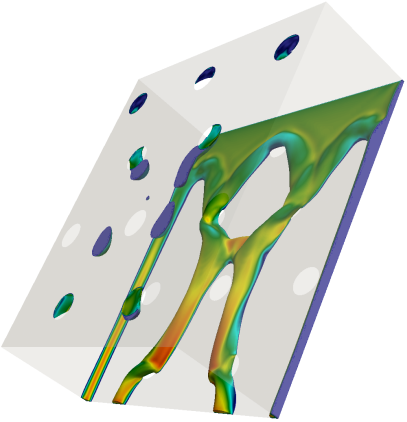


Test of perforation

Modeling of flow between two perforated plates

Example: $B = 40\,[\mathrm{m\,h^{-1}}]$, $d_{\mathrm{perf}} = 5\,[\mathrm{mm}]$

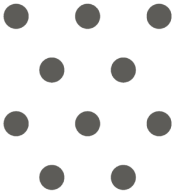


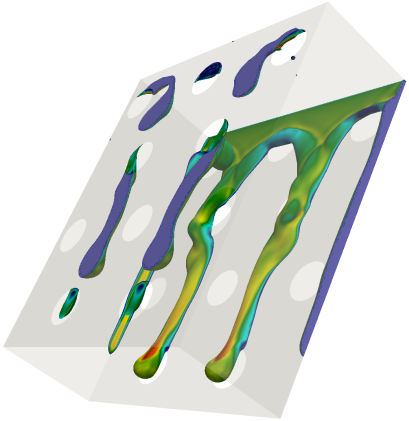


Test of perforation

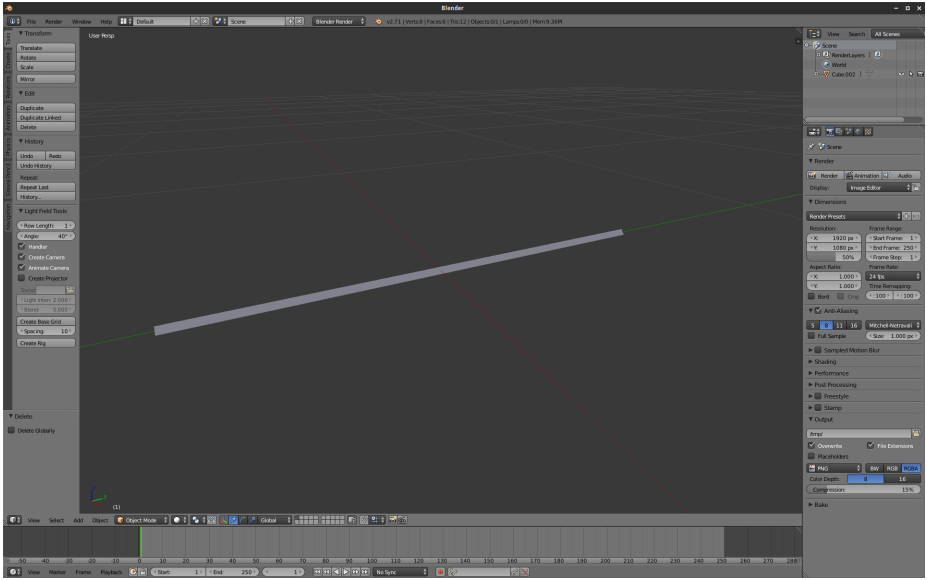
Modeling of flow between two perforated plates

Example: $B = 40\,[\mathrm{m\,h^{-1}}]$, $d_{\mathrm{perf}} = 7\,[\mathrm{mm}]$

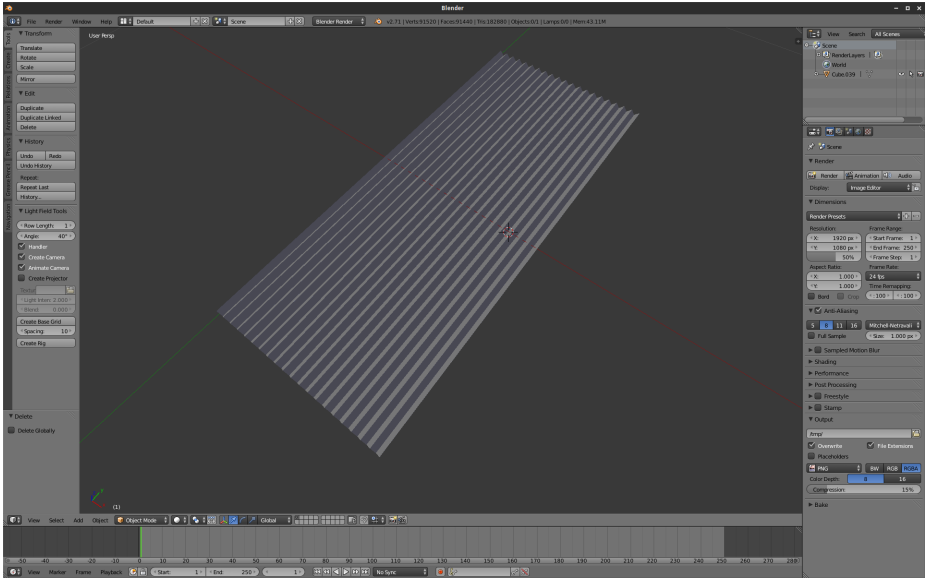




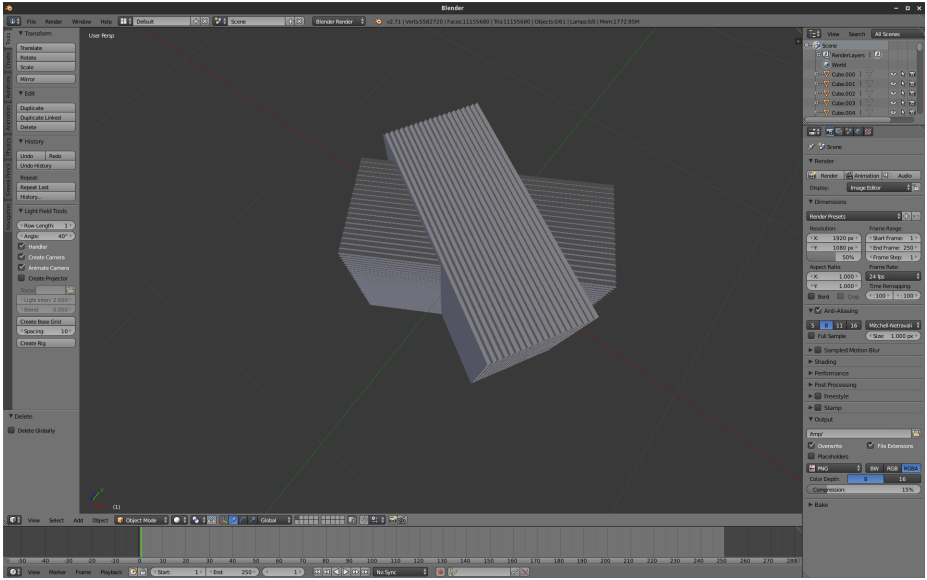
Step 1: Create base packing element



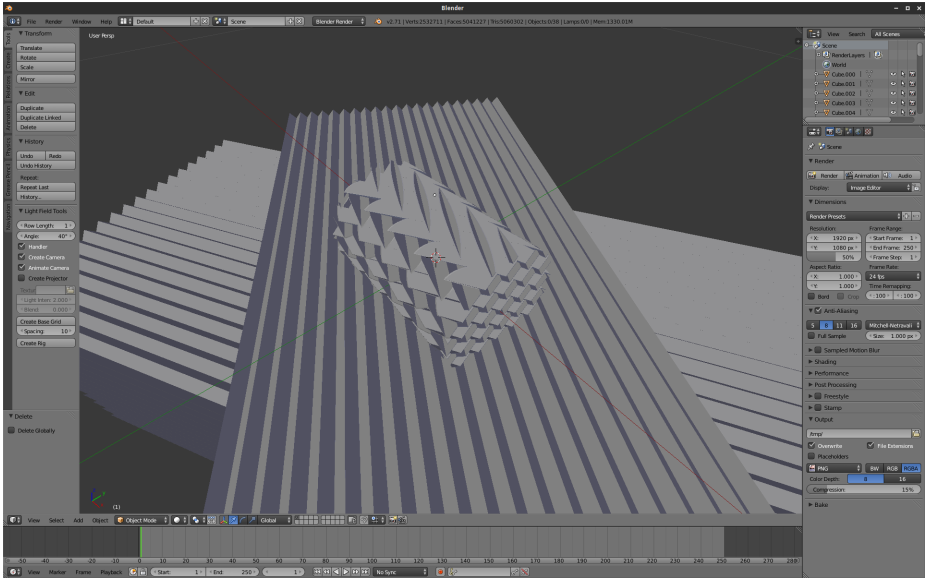
Step 2: Construct one corrugate sheet



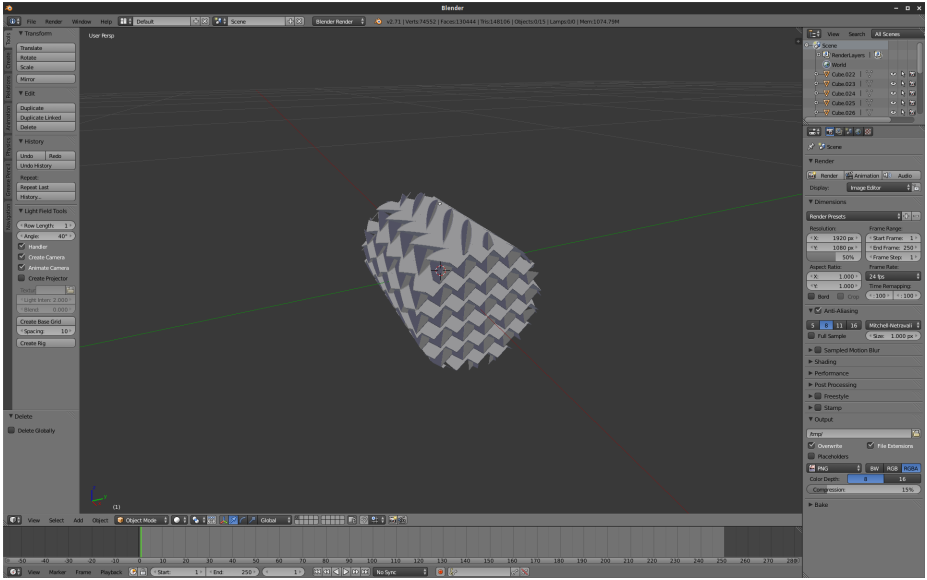
Step 3: Prepare all the needed sheet



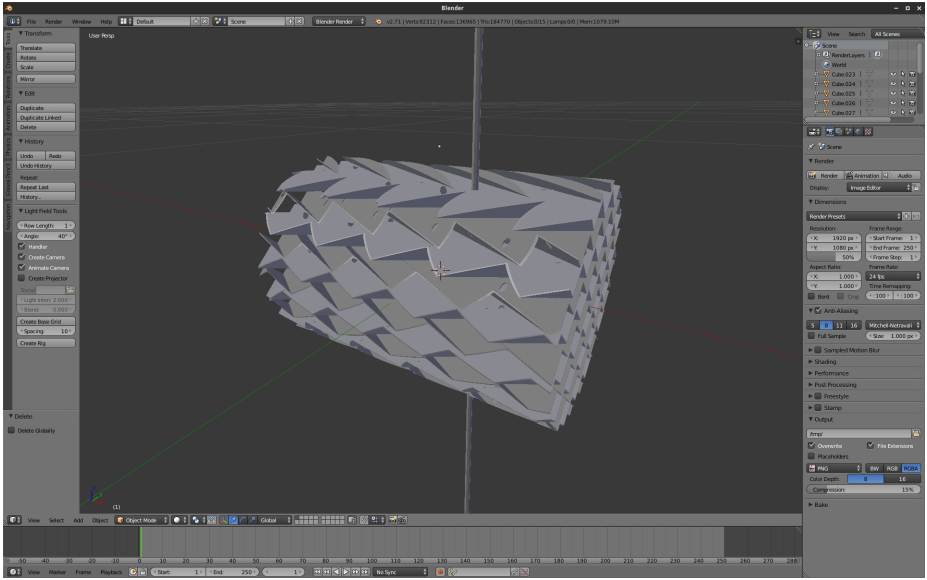
Step 4: Cut out the desired packing shape



Step 4: Cut out the desired packing shape



Step 5: Perforate the packing

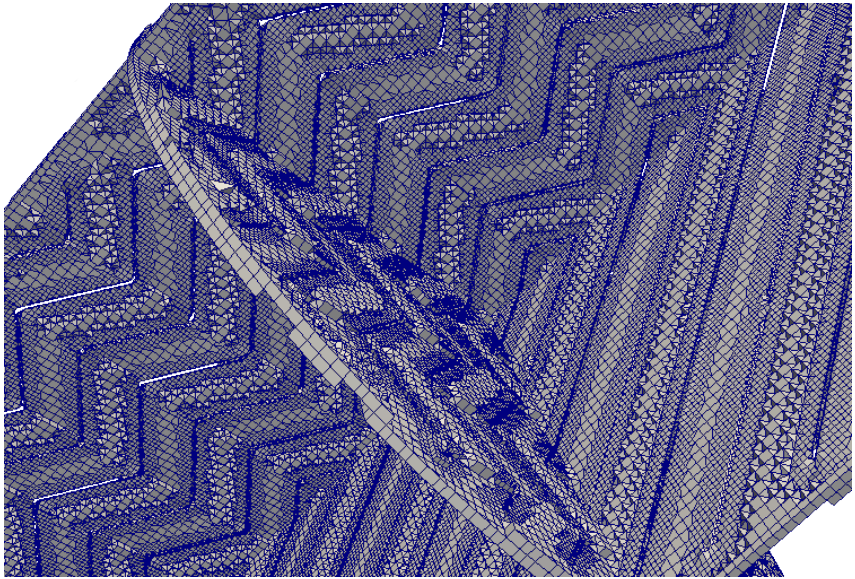


Step 6: Finish the packed bed generation

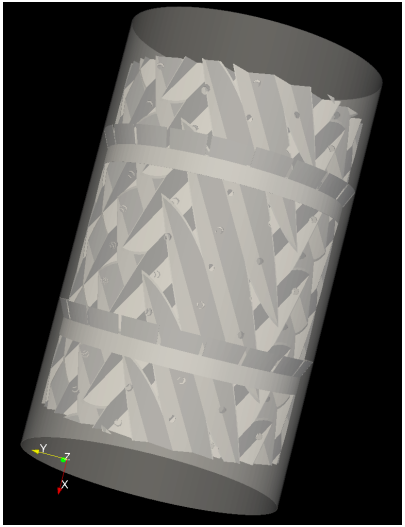
Geometry meshing

OpenFOAM core tool for FVM meshes generation – snappyHexMesh

Mesh: Unstructured, hex dominated, $\mathrm{nCells} \approx 10^6 - 10^7$/packing element



Testing: What can be actually measured



Pressure loss

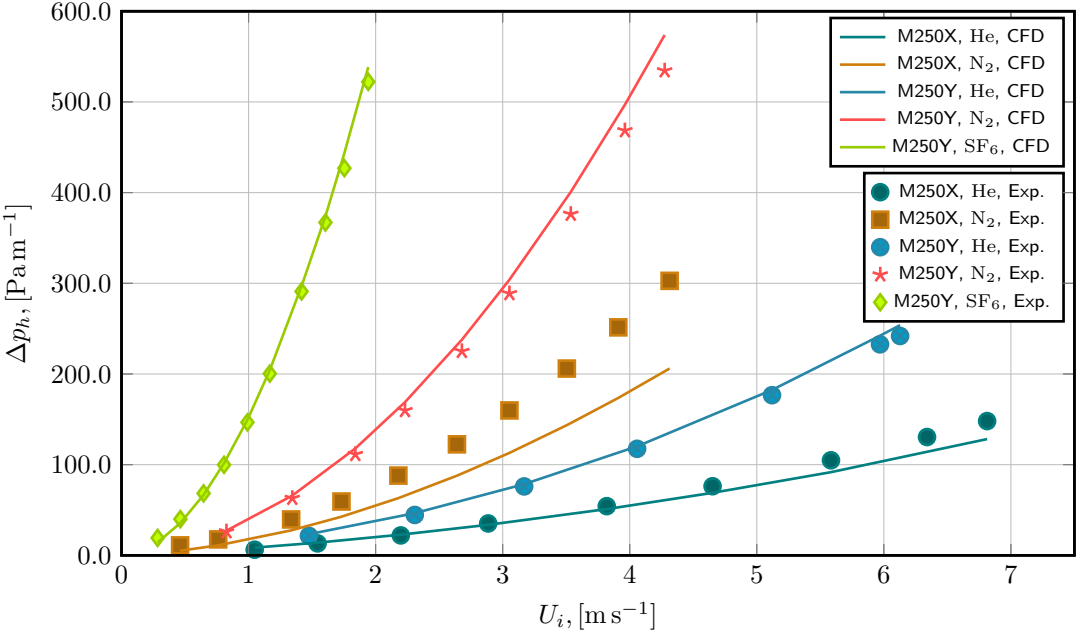
$$\Delta p_h := \frac{p_{\text{above}} - p_{\text{bellow}}}{N_{\text{pk}} H_{\text{pk}}}$$

Notations

$N_{\text{pk}}[-]$ ..... number of packing elements
$H_{\text{pk}}[\text{m}]$ ..... height of packing element

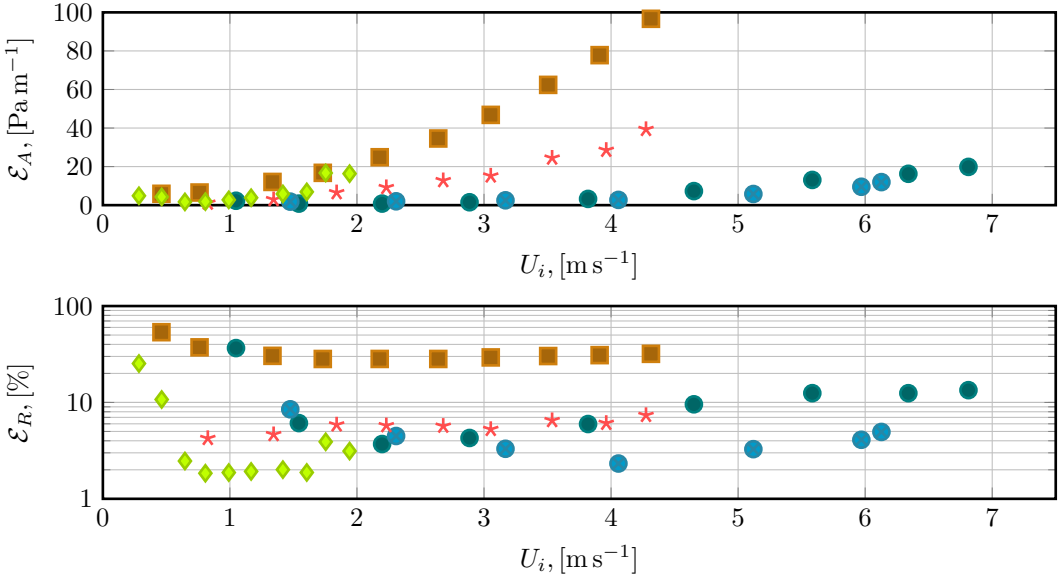
Single-phase testing

Evaluation of packing dry pressure loss [exp. by Haidl et al., UCT Prague]



Single-phase testing

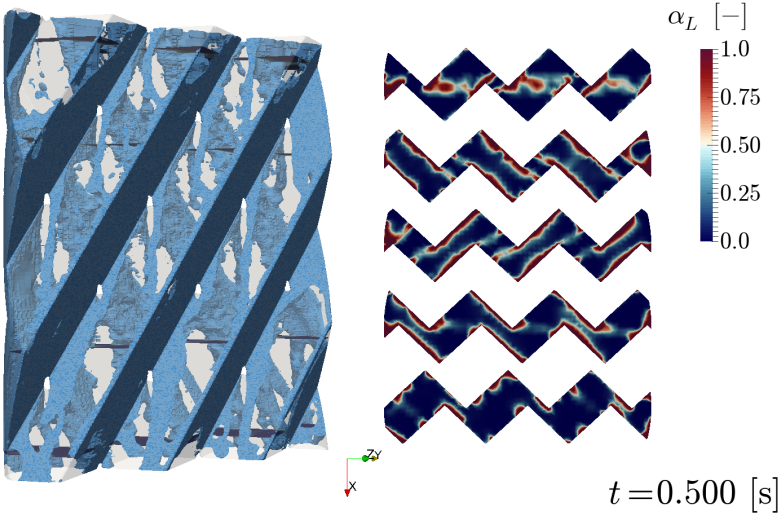
Evaluation of packing dry pressure loss [exp. by Haidl et al., UCT Prague]



Multiphase testing

Evaluation of interFoam stability (coarse mesh and extreme liquid flow rate)

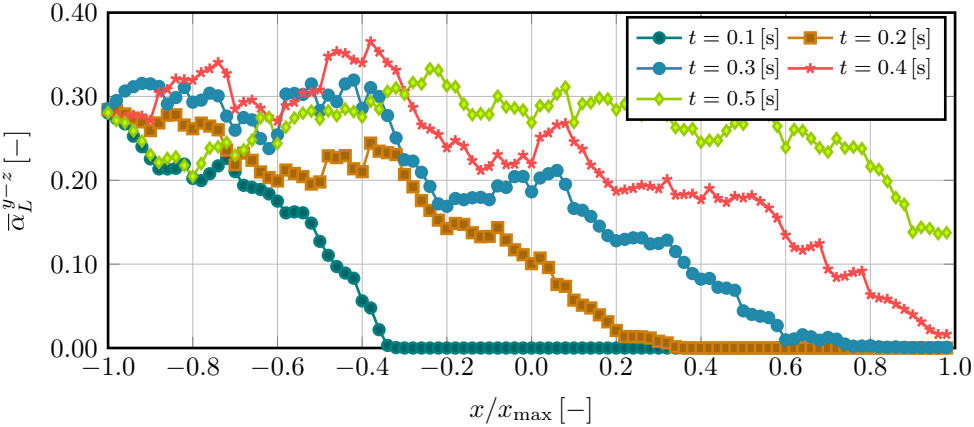
Superficial liquid velocity: $B = Q_{\mathrm{liquid}}/\mathrm{Area}(\text{geom. cross sec.}) = 200\,[\mathrm{m\,h^{-1}}]$



Liquid distribution in packing

Calculate "volume fraction" of liquid along the packing

Example: 100 slices in $y - z$ plane through geometry from previous slide



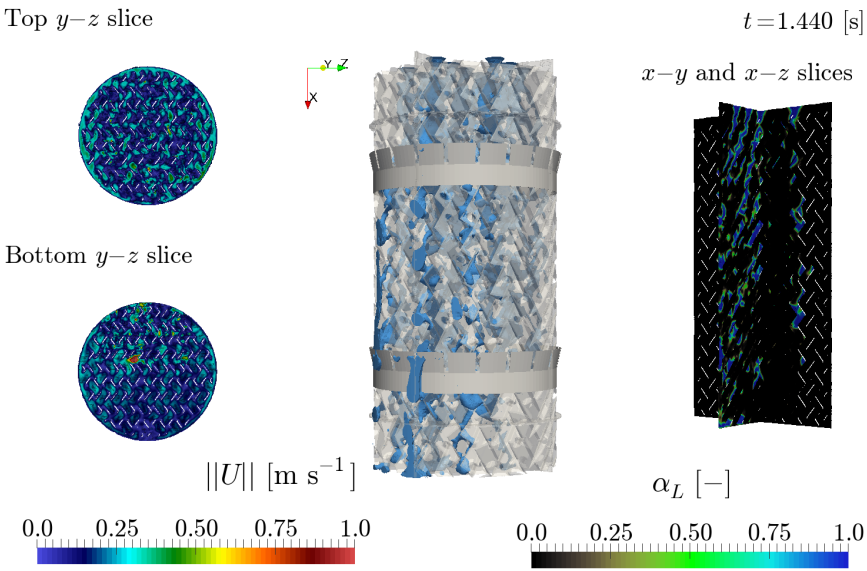
$$\overline{\alpha}_L^{y-z}(x_i) = \frac{1}{\eta^{y-z}(x_i)} \int_{\eta^{y-z}(x_i)} \alpha_L \, \mathrm{d}S, \; \eta^{y-z}(x_i) = \left\{ \mathbf{x} \in \Omega^h : x = x_i \right\}$$

Actual simulations

Auxiliary geometry

The original geometry is too big for testing simulations

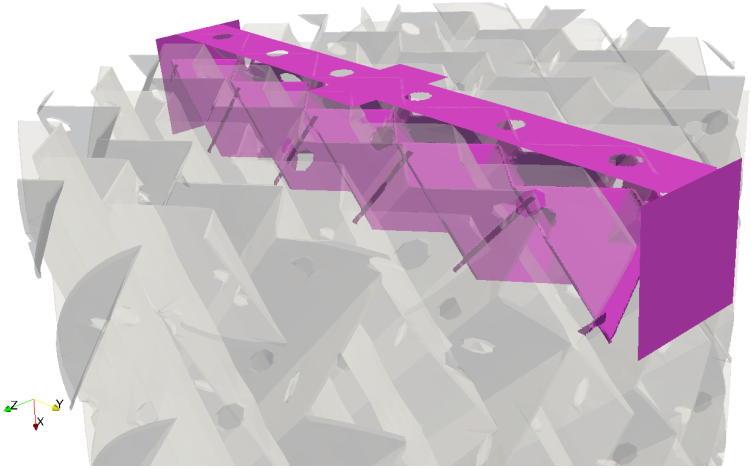
Original geometry: Cylinder $d_{\mathrm{col}} = 100 - 150\,[\mathrm{mm}]$, $h_{\mathrm{col}} = 210\,[\mathrm{mm}]$ $\rightsquigarrow$ to big for testing



Auxiliary geometry

The original geometry is too big for testing simulations

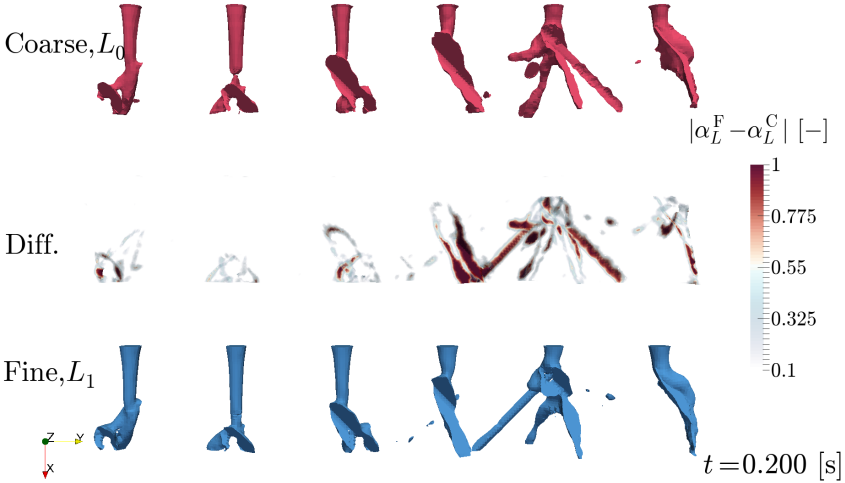
Auxiliary geometry: Hexaheder $\Delta x \times \Delta y \times \Delta z = 25 \times 150 \times 24\,[\mathrm{mm}] \rightsquigarrow$ used for mesh size independence study and testing of the basic flow behavior



Mesh size independence study

How fine mesh do we need or can afford?

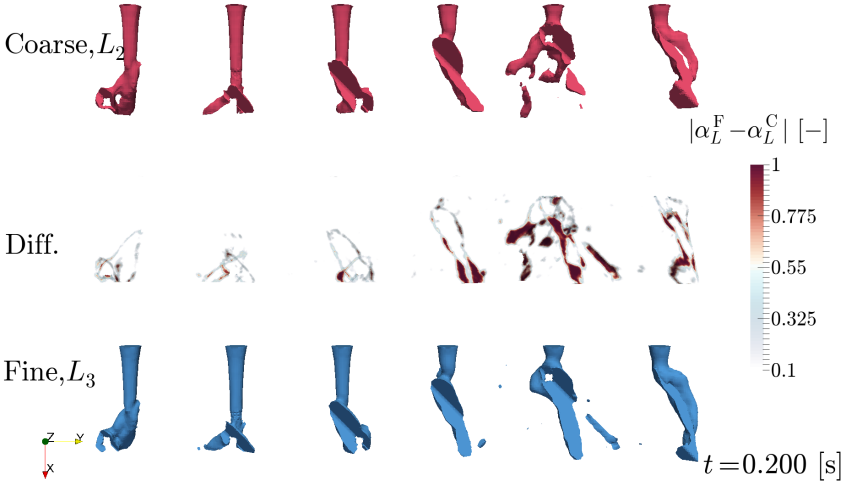
Qualitative comparison: L_0 mesh, $\approx 180 \cdot 10^3$ cells L_1 mesh, $\approx 350 \cdot 10^3$ cells



Mesh size independence study

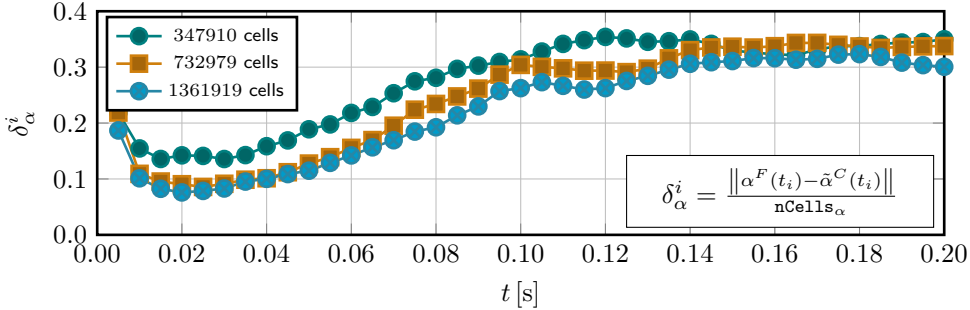
How fine mesh do we need or can afford?

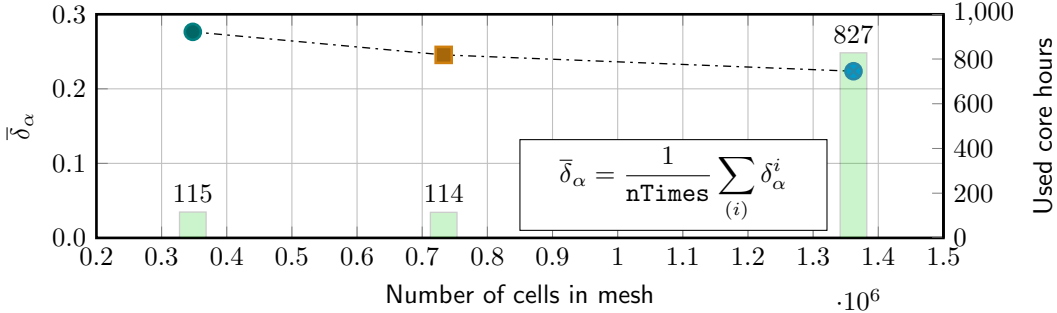
Qualitative comparison: L_2 mesh, $\approx 730 \cdot 10^3$ cells L_3 mesh, $\approx 1360 \cdot 10^3$ cells



Mesh size independence study

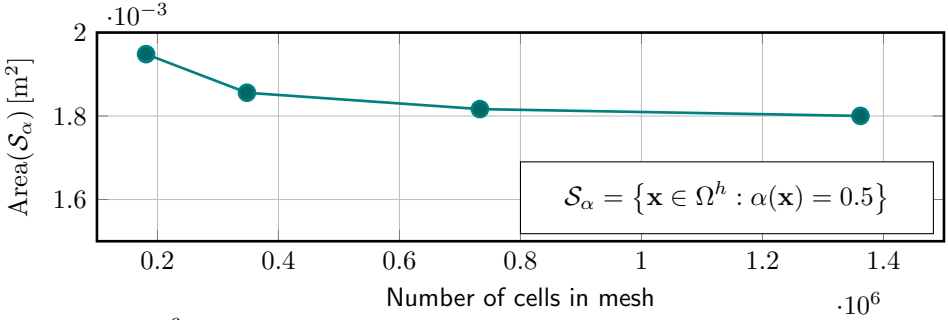
How fine mesh do we need or can afford?

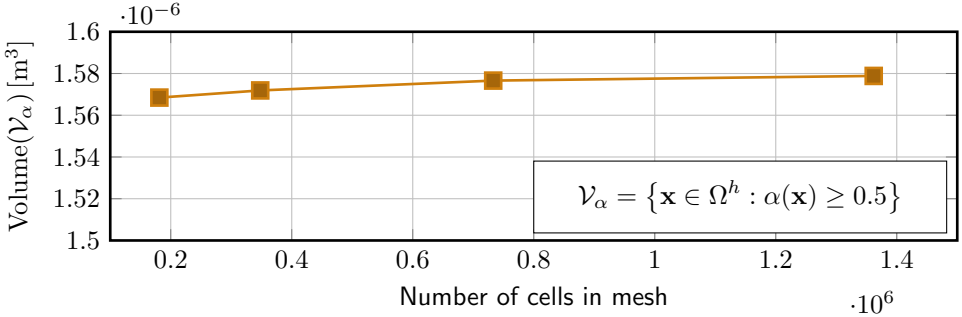




Mesh size independence study

How fine mesh do we need or can afford?



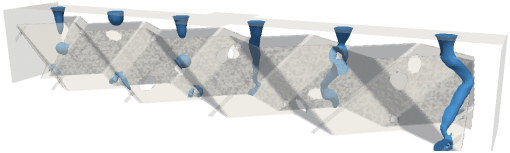


Testing of liquid behavior

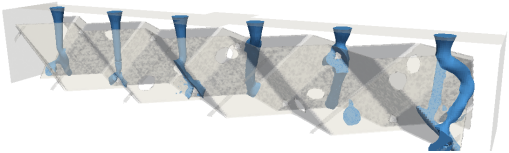
Focused at wetting for different liquid flow rates

Superficial liquid velocity: $B = Q_{\mathrm{liquid}}/\mathrm{Area}(\text{geom. cross sec.})\,[\mathrm{m\,h^{-1}}]$

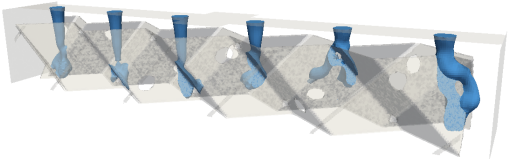
$B = 5\,[\mathrm{m\,h^{-1}}]$



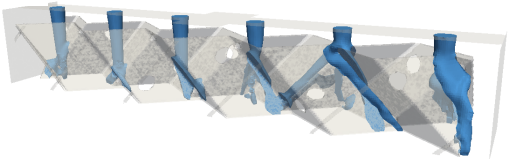
$B = 10\,[\mathrm{m\,h^{-1}}]$



$B = 20\,[\mathrm{m\,h^{-1}}]$



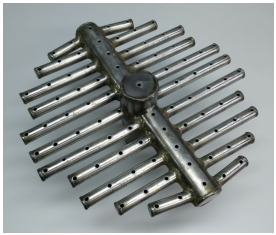
$B = 40\,[\mathrm{m\,h^{-1}}]$



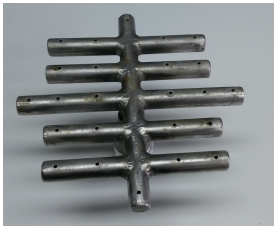
Standard liquid inlet

Shower-like device to "evenly" distribute liquid on column top

Real life liquid inlet



$d_{\mathrm{col}} = 300\,[\mathrm{mm}]$



$d_{\mathrm{col}} = 150\,[\mathrm{mm}]$

[Mass trasfer lab. at UCT Prague]

OpenFOAM approximation

$d_{\mathrm{col}} = 100\,[\mathrm{mm}]$

Standard liquid inlet

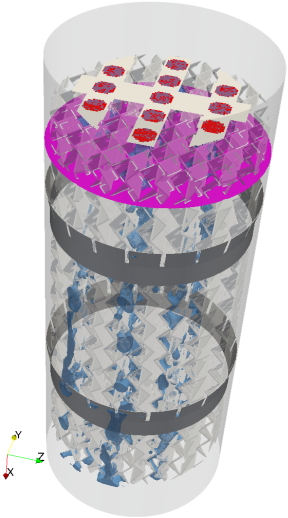
Shower-like device to "evenly" distribute liquid on column top

Advantages

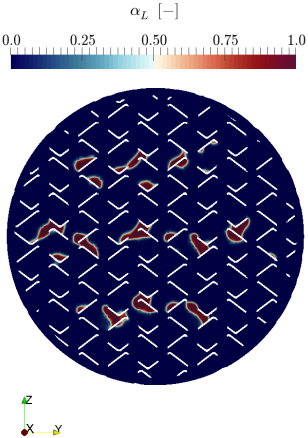
- Corresponds to the actually used inlet

Disadvantages

- Poor liquid distribution
- Simulation of 1 PE $\approx$ simulation of the topmost PE $\implies$ irrelevant during standard operation

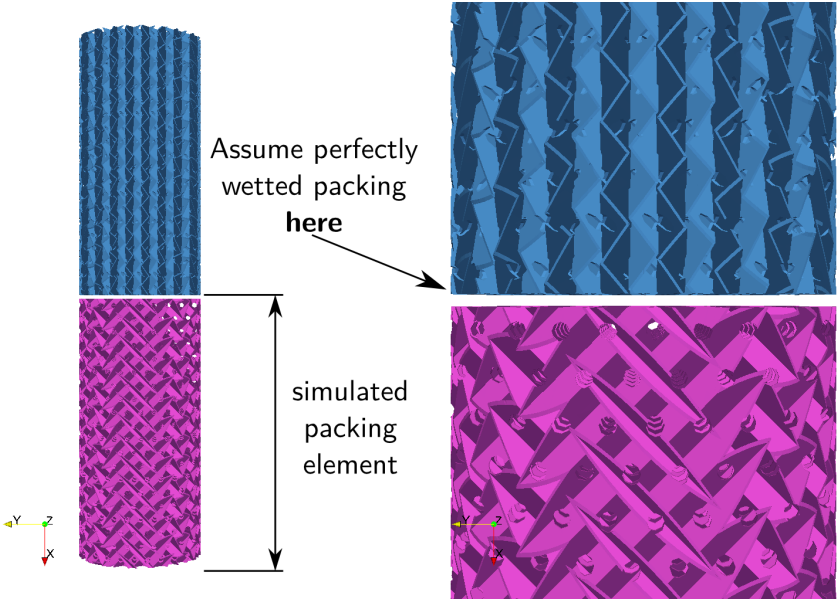


Example of liquid distribution



Simulation of ideal liquid distribution

Assume even liquid distribution on the whole packing



Simulation of ideal liquid distribution

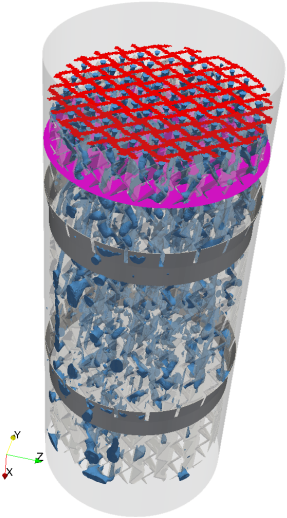
Assume even liquid distribution on the whole packing

Advantages

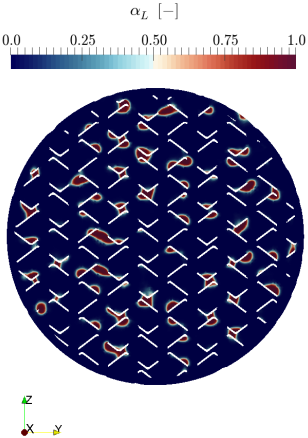
- Improved liquid distribution
- "Mid-column conditions"

Disadvantages

- Longer simulation times
- Less stable

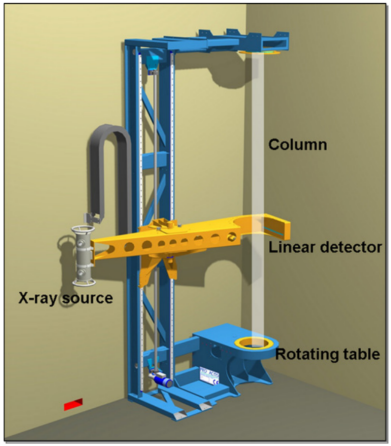


Example of liquid distribution



Available experimental data
Usage of 3D X-Ray Tomography

Experimental device: [S. Aferka et al., Tomographic measurement of liquid hold up and effective interfacial area distributions in a column packed with high performance structured packings. *Chem. Eng. Sci.*, 66:3414–3422, 2011.]



Operation:

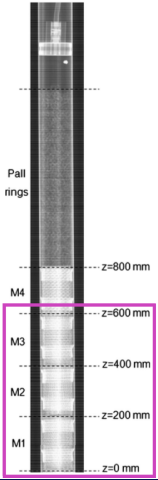
- Static X-Ray
- Rotating column

Characteristics:

- Packing: MellapakPlus 752.Y
- $d_{\mathrm{col}} = 100\,[\mathrm{mm}]$
- $h_{\mathrm{bed}} = 800\,[\mathrm{mm}]$, 4 pack. el.
- Rotation time/360°: $45 - 180\,[\mathrm{s}]$

Available experimental data
Usage of 3D X-Ray Tomography

Experimental device: [S. Aferka et al., Tomographic measurement of liquid hold up and effective interfacial area distributions in a column packed with high performance structured packings. *Chem. Eng. Sci.*, 66:3414–3422, 2011.]



Elements of interest

Operation:

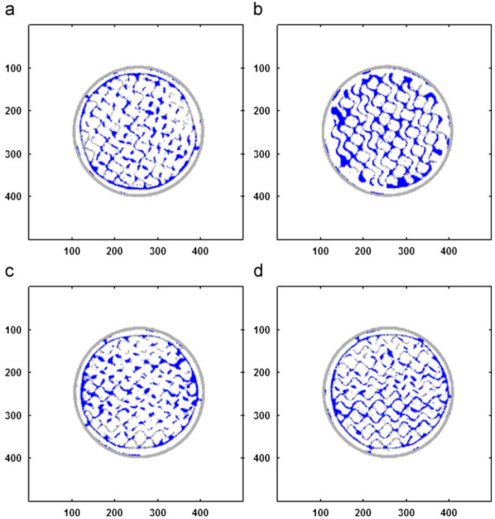
- Static X-Ray
- Rotating column

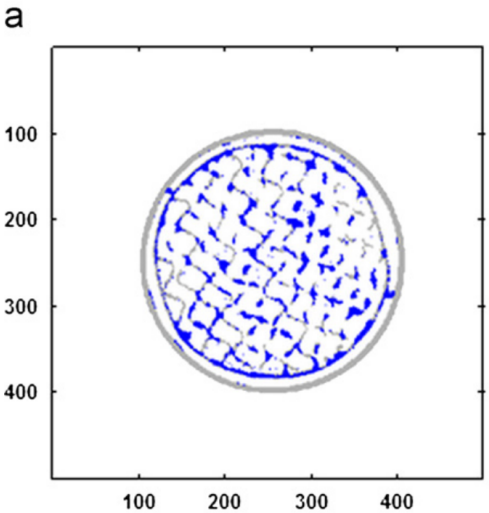
Characteristics:

- Packing: MellapakPlus 752.Y
- $d_{\mathrm{col}} = 100\,[\mathrm{mm}]$
- $h_{\mathrm{bed}} = 800\,[\mathrm{mm}]$, 4 pack. el.
- Rotation time/360°: $45 - 180\,[\mathrm{s}]$

Available experimental data
Usage of 3D X-Ray Tomography

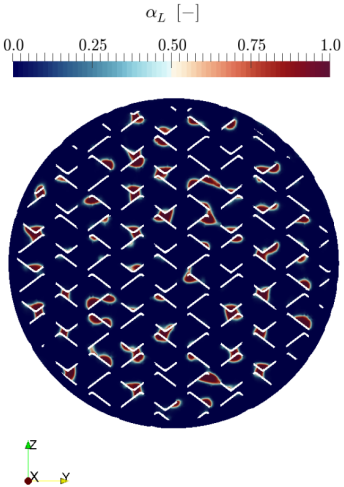
Experimental data: Liquid distribution along the column, 500, 600, 700 and $800\,[\mathrm{mm}]$ from the column bottom, $B = 23.1\,[\mathrm{m\,h^{-1}}]$, MP752Y [S. Aferka et al. *Chem. Eng. Sci.*, 2011.]

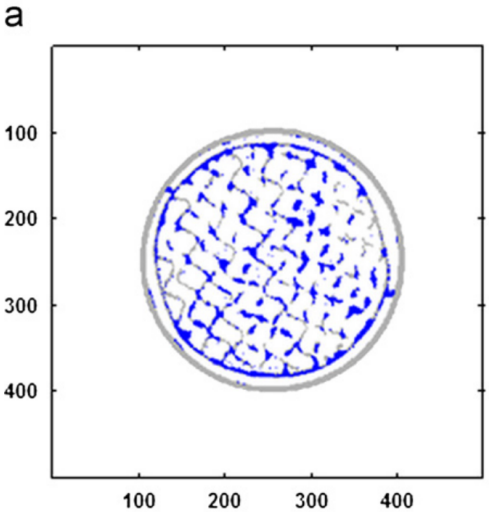




Available experimental data
Usage of 3D X-Ray Tomography

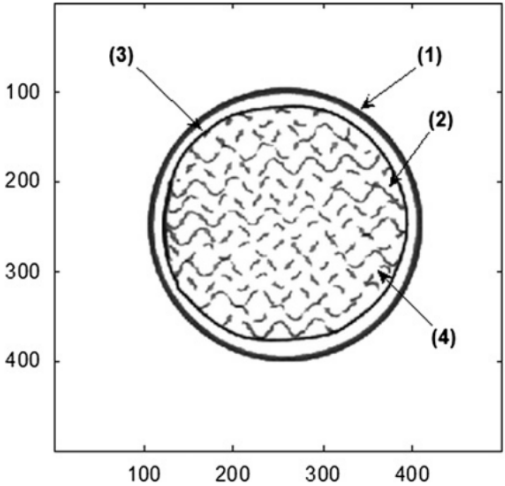
Experimental data: Liquid distribution along the column, 500, 600, 700 and $800\,[\mathrm{mm}]$ from the column bottom, $B = 23.1\,[\mathrm{m\,h^{-1}}]$, MP752Y [S. Aferka et al. *Chem. Eng. Sci.*, 2011.]





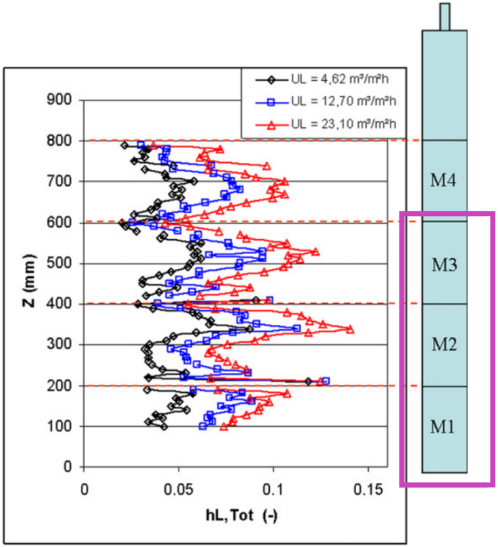
Available experimental data
Usage of 3D X-Ray Tomography

Experimental data: Liquid distribution along the column, 500, 600, 700 and $800\,[\mathrm{mm}]$ from the column bottom, $B = 23.1\,[\mathrm{m\,h^{-1}}]$, MP752Y [S. Aferka et al. *Chem. Eng. Sci.*, 2011.]



Available experimental data
Usage of 3D X-Ray Tomography

Experimental data: Liquid distribution along the column, 500, 600, 700 and $800\,[\mathrm{mm}]$ from the column bottom, $B = 23.1\,[\mathrm{m\,h^{-1}}]$, MP752Y [S. Aferka et al. *Chem. Eng. Sci.*, 2011.]

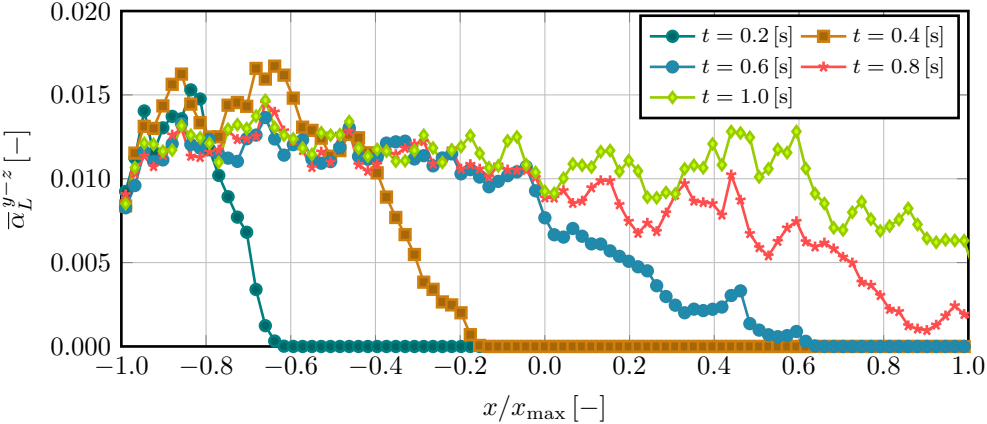


Elements of interest

Liquid distribution in packing

Calculate "volume fraction" of liquid along the packing

Example: MP250X packing, $d_{\mathrm{col}} = 150\,[\mathrm{mm}]$, $H_{\mathrm{pkg}} = 200\,[\mathrm{mm}]$, $B = 10.2\,[\mathrm{m\,h^{-1}}]$, 100 slices along x coordinate, old inlet

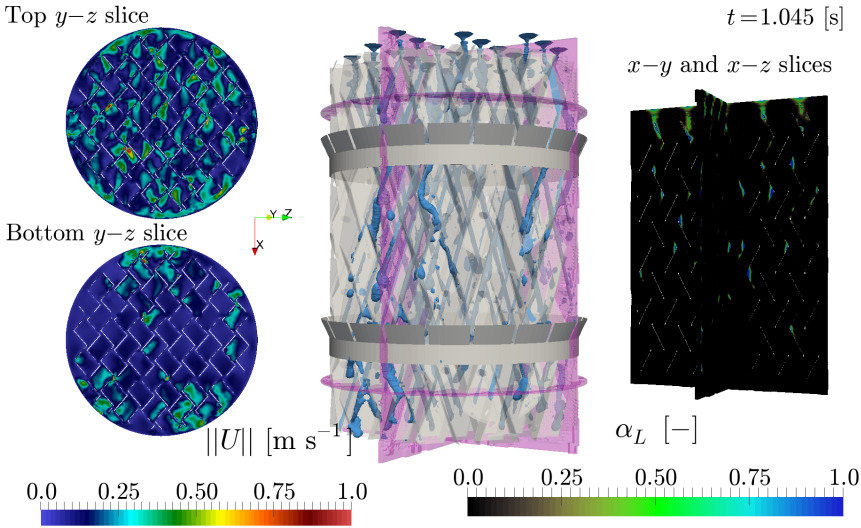


$$\overline{\alpha}_L^{y-z}(x_i) = \frac{1}{\eta^{y-z}(x_i)} \int_{\eta^{y-z}(x_i)} \alpha_L \,\mathrm{d}S,\ \eta^{y-z}(x_i) = \left\{\mathbf{x} \in \Omega^h : x = x_i\right\}$$

Liquid distribution in packing

Calculate "volume fraction" of liquid along the packing

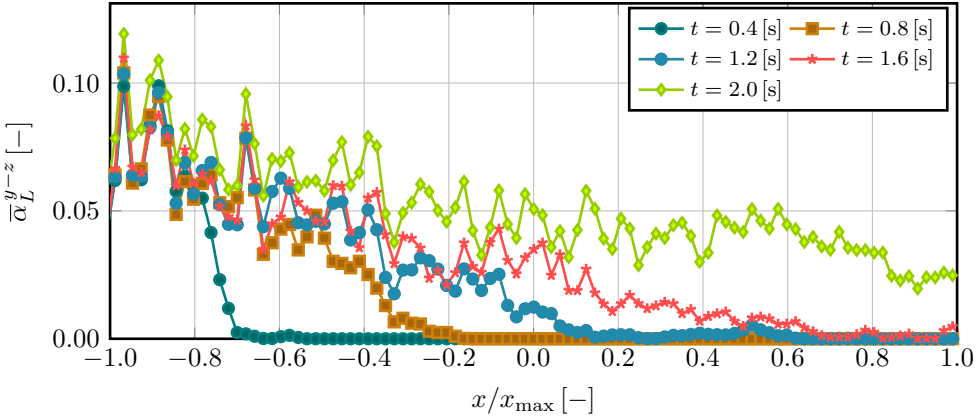
Example: MP250X packing, $d_{\mathrm{col}} = 150\,[\mathrm{mm}]$, $H_{\mathrm{pkg}} = 200\,[\mathrm{mm}]$, $B = 10.2\,[\mathrm{m\,h^{-1}}]$, 100 slices along x coordinate, old inlet



Liquid distribution in packing

Calculate "volume fraction" of liquid along the packing

Example: MP750Y packing, $d_{\mathrm{col}} = 100\,[\mathrm{mm}]$, $H_{\mathrm{pkg}} = 200\,[\mathrm{mm}]$, $B = 23.1\,[\mathrm{m\,h^{-1}}]$, 100 slices along x coordinate

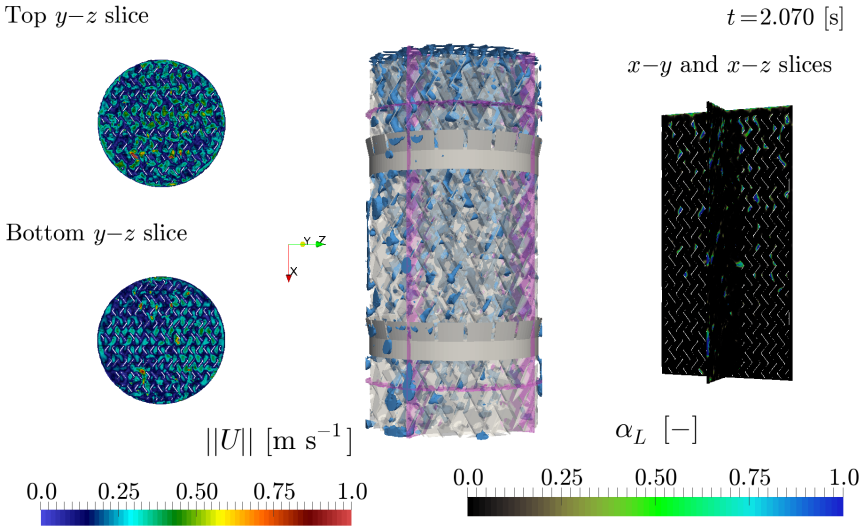


$$\overline{\alpha}_L^{y-z}(x_i) = \frac{1}{\eta^{y-z}(x_i)} \int_{\eta^{y-z}(x_i)} \alpha_L \,\mathrm{d}S,\ \eta^{y-z}(x_i) = \left\{\mathbf{x} \in \Omega^h : x = x_i\right\}$$

Liquid distribution in packing

Calculate "volume fraction" of liquid along the packing

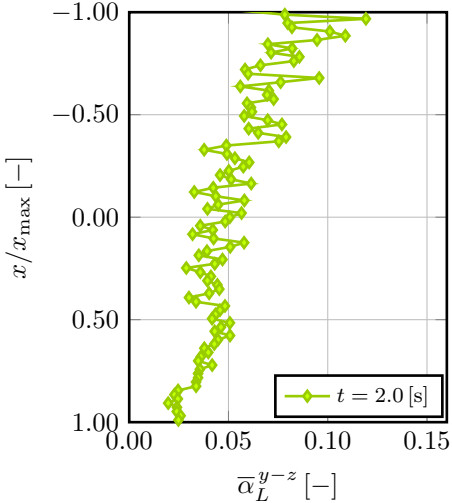
Example: MP750Y packing, $d_{\mathrm{col}} = 100\,[\mathrm{mm}]$, $H_{\mathrm{pkg}} = 200\,[\mathrm{mm}]$, $B = 23.1\,[\mathrm{m\,h^{-1}}]$, 100 slices along x coordinate

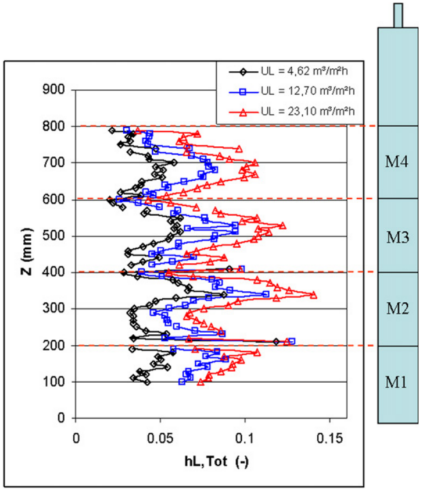


Liquid distribution in packing

Calculate "volume fraction" of liquid along the packing

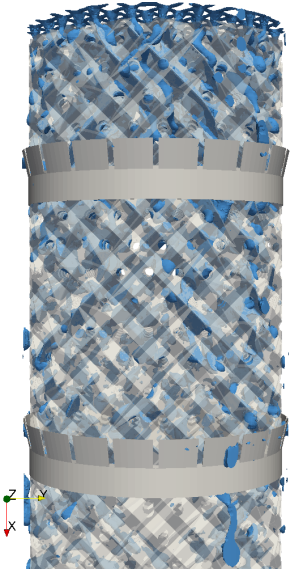
Example: MP750Y packing, $d_{\mathrm{col}} = 100\,[\mathrm{mm}]$, $H_{\mathrm{pkg}} = 200\,[\mathrm{mm}]$, $B = 23.1\,[\mathrm{m\,h^{-1}}]$, 100 slices along x coordinate

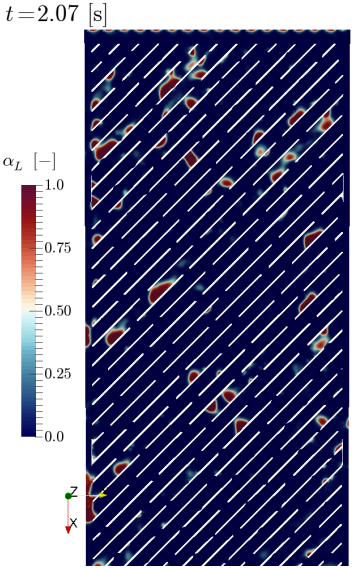




Liquid distribution in packing

Qualitative exploration of liquid distribution





Conclusions

Currently available

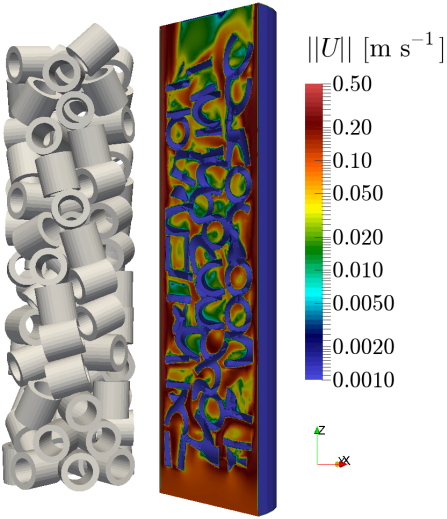
- Single phase steady state simulations $\rightsquigarrow$ dry pressure loss estimation
- Multiphase simulations (limited dataset)

Next steps

- Finish the multiphase simulations
- Compare liquid hold up with experimental data
- Calculate wet pressure loss (moderate gas flow rates) and compare it with experimental data

Other research branches
Testing different types of packing

Random packings



Superpak packing

Acknowledgments

This work was supported by The Ministry of Education, Youth and Sports from the Large Infrastructures for Research, Experimental Development and Innovations project IT4Innovations National Supercomputing Center– LM2015070.

The work of M. Isoz was supported by the Centre of Excellence for nonlinear dynamic behaviour of advanced materials in engineering CZ.02.1.01/0.0/0.0/15_003/0000493 (Excellent Research Teams) in the framework of Operational Programme Research, Development and Education.

Special thanks to the Mass Transfer Research Group of the University of Chemistry and Technology in Prague for providing an acces to their experimental equipment as for as for many helpfull consults.

References

[1] Haroun, Y. Raynal, L.: Use of computational fluid dynamics for absorption packed column design. *Oil Gas Sc. Technol.*, 71:18, 2016.

[2] Owens, S. A. Perkins, M. R. Eldridge, R. B. Schulz K. W. Ketcham, R. A.: Computational fluid dynamics simulation of structured packing. *Ind. Eng. Chem Res.*, 52:2032–2045, 2013.

[3] Amini, Y. Karimi-Sabet, J. Esfahany, M. N.: Experimental and numerical simulation of dry pressure drop in high-capacity structured packings. *Chem. Eng. Technol.*, 39:1161–1170, 2016.

[4] Khosravi-Nikou, M. R. Eshani, M. R.: Turbulence models application on CFD simulation of hydrodynamics heat and mass transfer in structured packing. *Int. Comm. Heat Mass Tr.*, 17:21, 2008.

[5] Marchot, P. Toye, D. Pelsser, A. M., L'Homme, G. Olujic, Z.: Liquid distribution images on structured packing by X-Ray computed tomography. *AIChE J.*, 47:1471–1476, 2001.

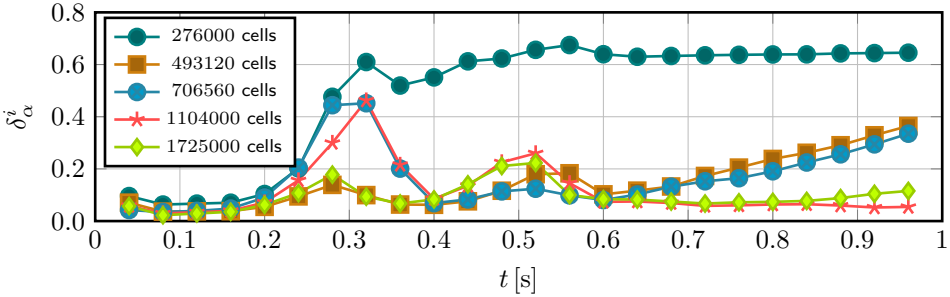
[6] Aferka, S. et al.: Tomographic measurement of liquid hold up and effective interfacial area distributions in a column packed with high performance structured packings. *Chem. Eng. Sci.*, 66:3414–3422, 2011.

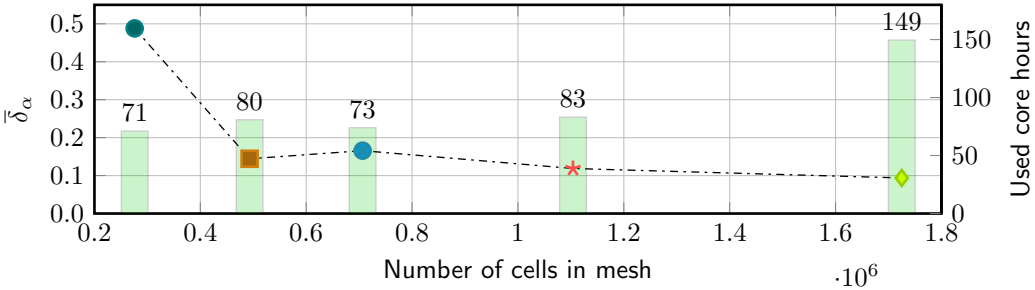
[7] Basden, M. et al.: Liquid holdup profiles in structured packing determined via neutron radiography. *Ind. Eng. Chem. Res.*, 52:17263–17269, 2013.

Thank you for your attention

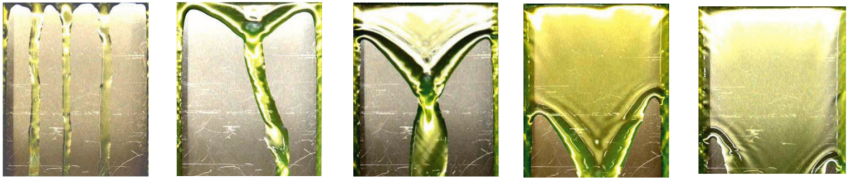
Microscale simulations

Mesh size independence study - transversal texture



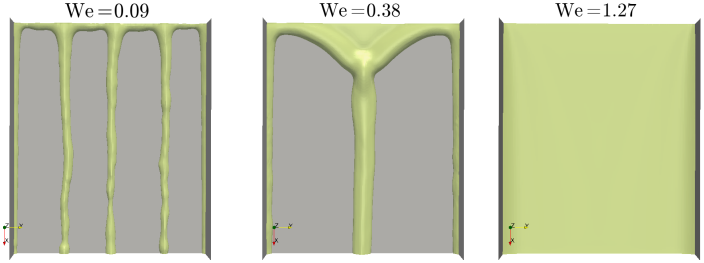


Wetted to total area ratio: Flow regimes in dependence on We



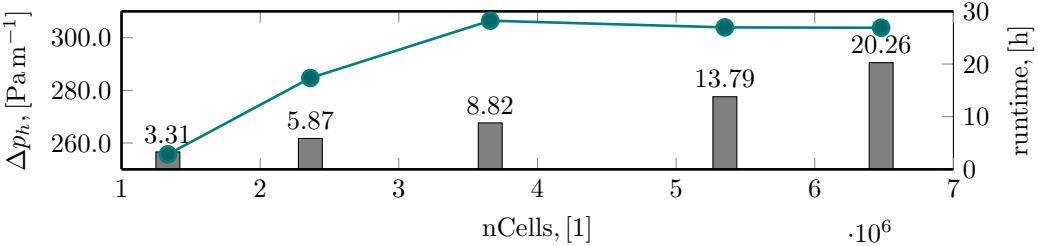
(a) $\mathrm{We}_{l\,\mathrm{N}}$ =0.05 (b) $\mathrm{We}_{l\,\mathrm{N}}$ =0.33 (c) $\mathrm{We}_{l\,\mathrm{N}}$ =0.73 (d) $\mathrm{We}_{l\,\mathrm{N}}$ =1.01 (e) $\mathrm{We}_{l\,\mathrm{N}}$ =1.32

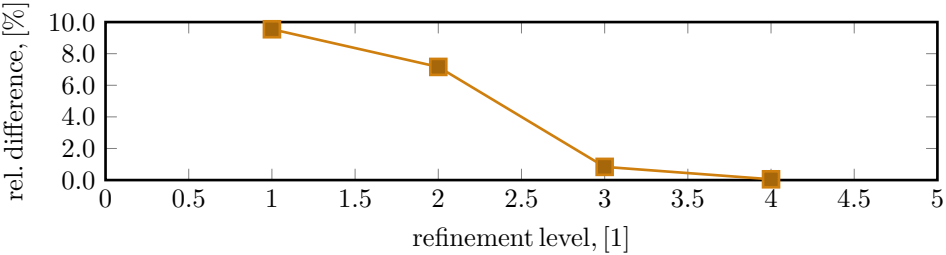
[Yoshiuki I. et al. Numerical and experimental study on liquid film flows on packing elements in absorbers for post-combustion CO_2 capture, *Energy Procedia*, **2013**]



Single phase model – mesh size determination

Main variable of interest is dry pressure loss, Δp_h

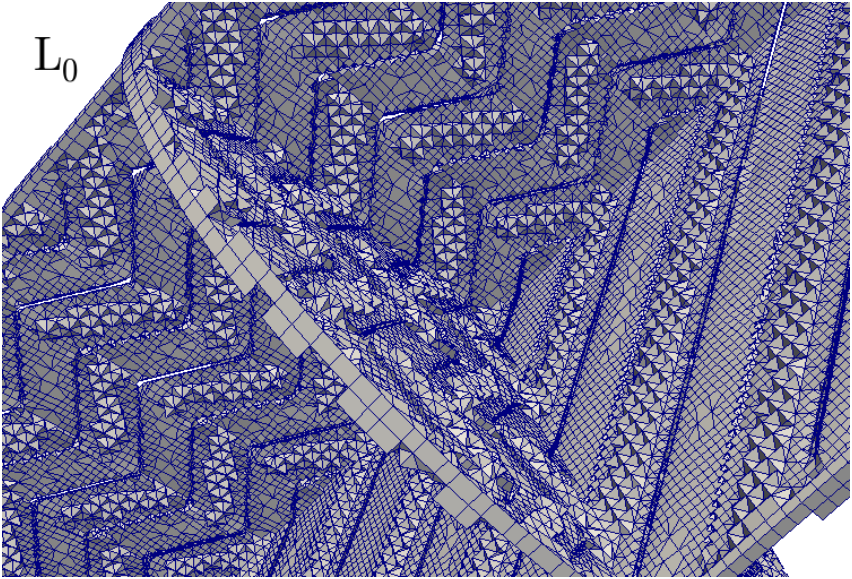




Single phase model – mesh size determination

Main variable of interest is dry pressure loss, Δp_h

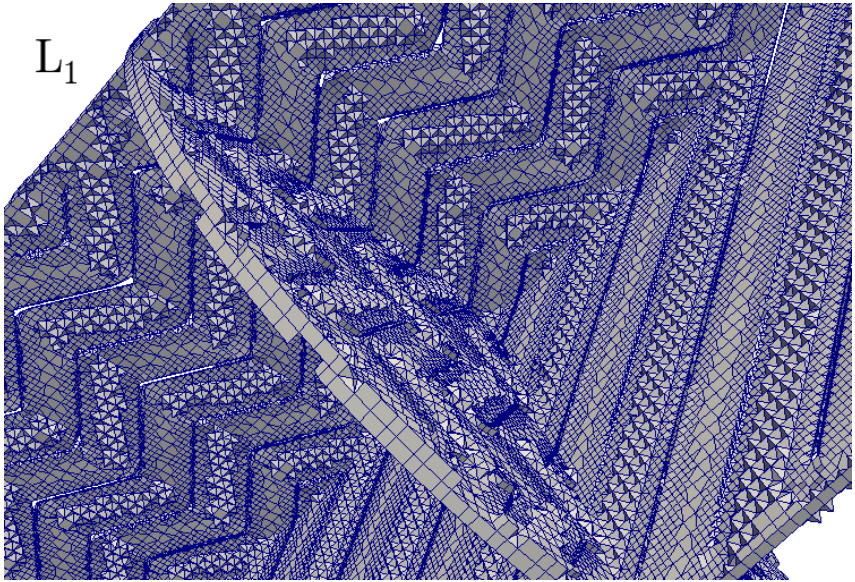
Mesh sizes: Mesh with $\mathrm{nCells} \approx 1 \cdot 10^6$/packing element



Single phase model – mesh size determination

Main variable of interest is dry pressure loss, Δp_h

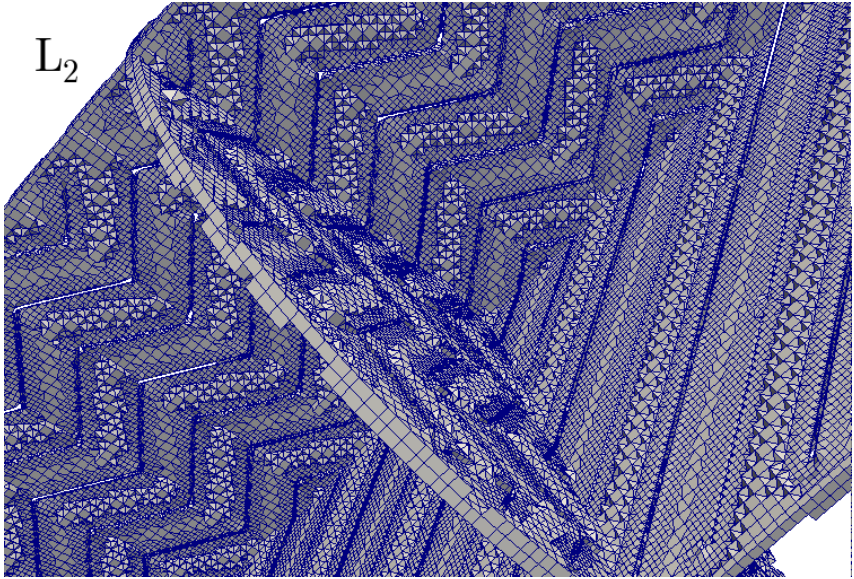
Mesh sizes: Mesh with $\mathrm{nCells} \approx 2.5 \cdot 10^6$/packing element



Single phase model – mesh size determination

Main variable of interest is dry pressure loss, Δp_h

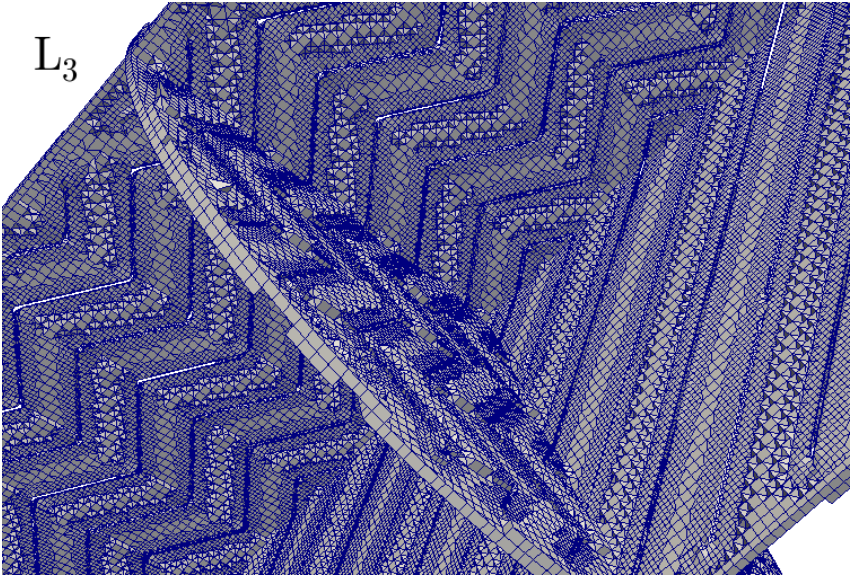
Mesh sizes: Mesh with $\mathrm{nCells} \approx 3.8 \cdot 10^6$/packing element



Single phase model – mesh size determination

Main variable of interest is dry pressure loss, Δp_h

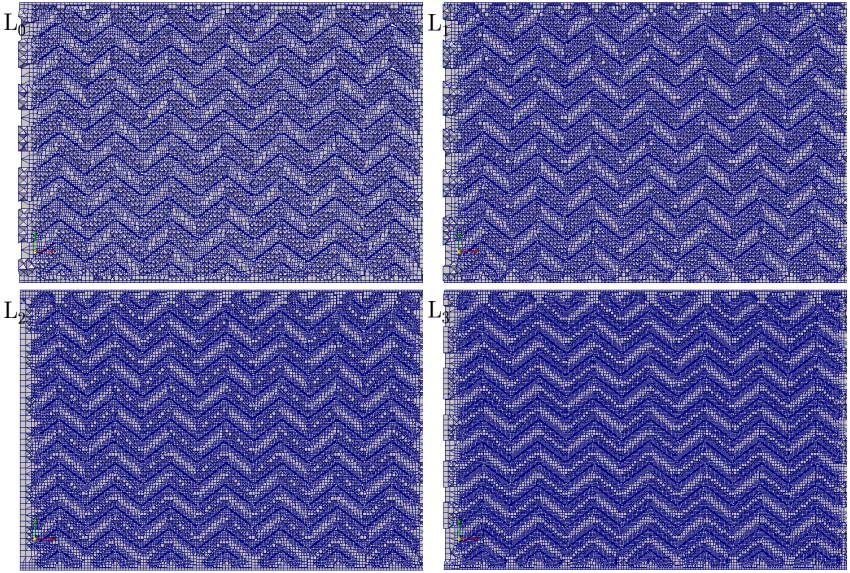
Mesh sizes: Mesh with $\mathrm{nCells} \approx 5.3 \cdot 10^6$/packing element



Single phase model – mesh size determination

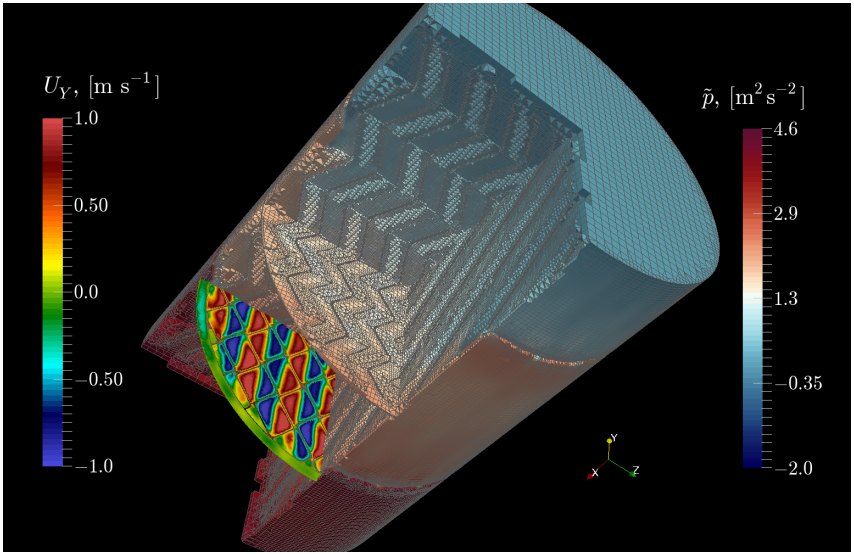
Main variable of interest is dry pressure loss, Δp_h

Mesh sizes: Side view on mesh levels $0 - 3$



Single phase model – model results
Pressure and velocity fields

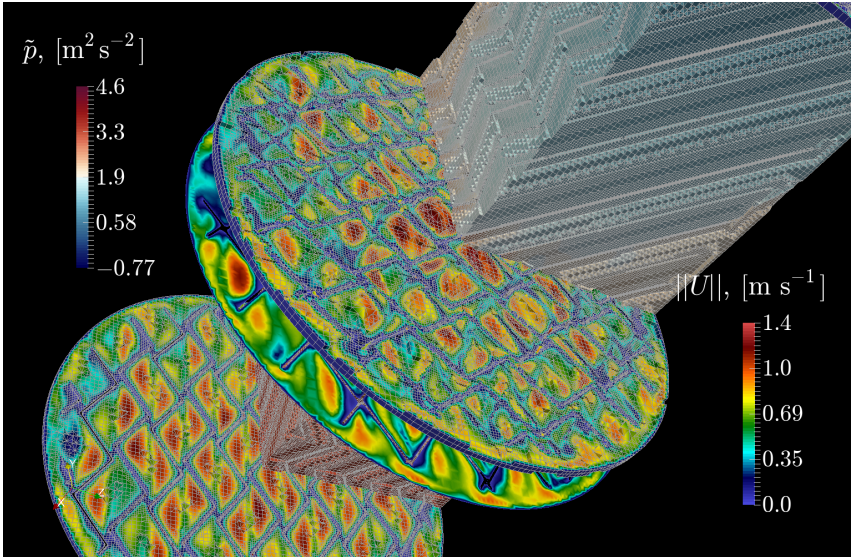
Result: flow patterns in 1 packing packing element



Single phase model – flow in two packing elements

Flow keeps its structure in most of the packing

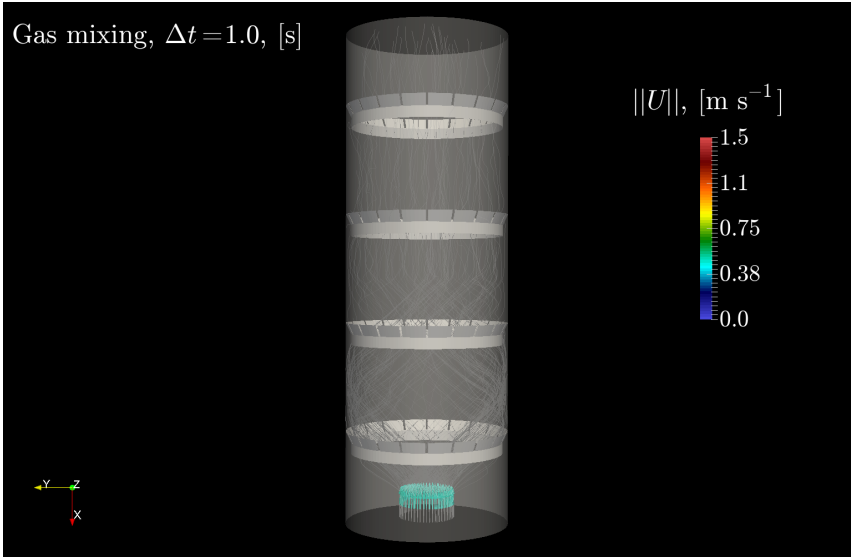
Simulation: Change of flow at transition between packing elements



Single phase model – mellapak packing mixing properties

Gas mixing in two packing elements

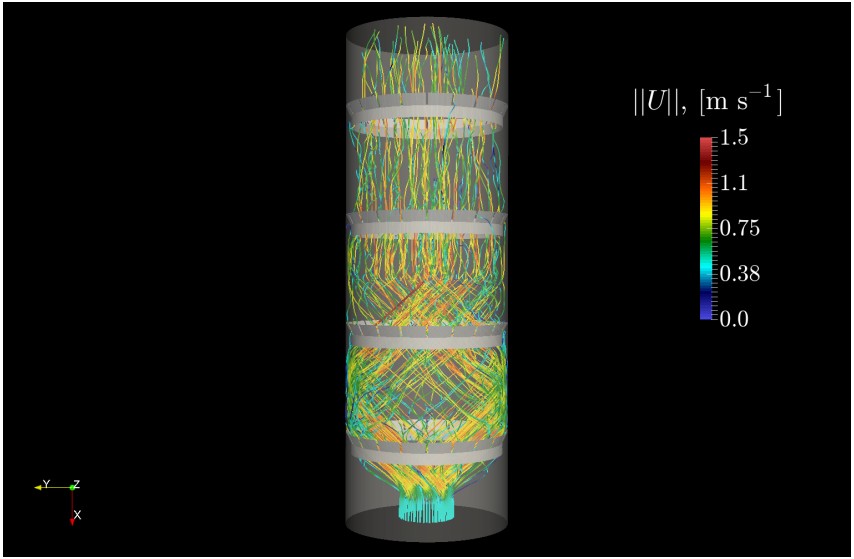
Seed: $\sigma_1 = \{(x, y, z) \in \mathcal{S} : x = -0.22\,\mathrm{m}, y^2 + z^2 \leq 0.025^2\,\mathrm{m}\}$



Single phase model – mellapak packing mixing properties

Gas mixing in two packing elements

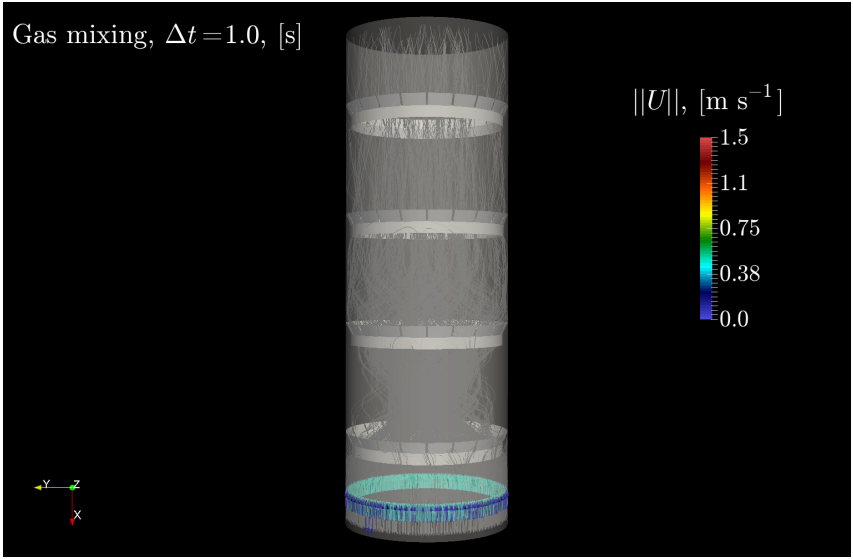
Seed: $\sigma_1 = \{(x, y, z) \in \mathcal{S} : x = -0.22\,\mathrm{m}, y^2 + z^2 \leq 0.025^2\,\mathrm{m}\}$



Single phase model – mellapak packing mixing properties

Gas mixing in two packing elements

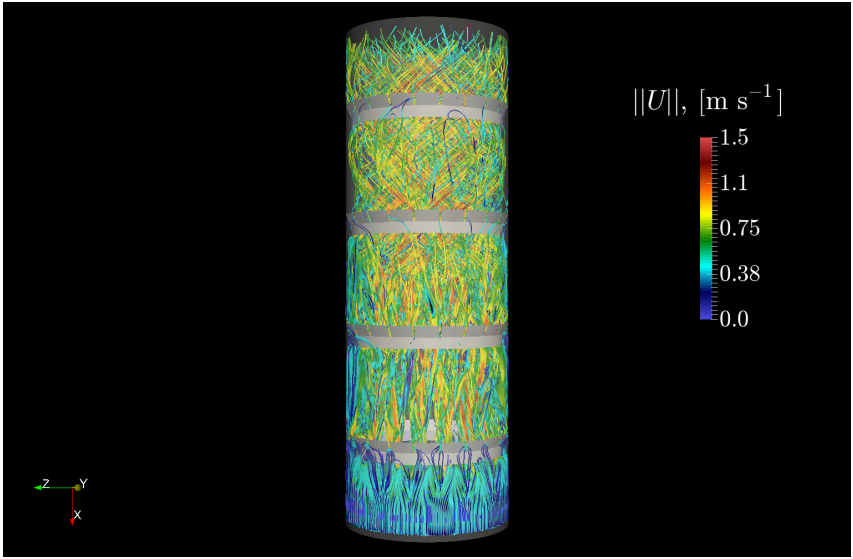
Seed: $\sigma_2 = \{(x, y, z) \in \mathcal{S} : x = -0.22\text{m}, 0.07^2\text{m} \leq y^2 + z^2 \leq 0.075^2\text{m}\}$



Single phase model – mellapak packing mixing properties

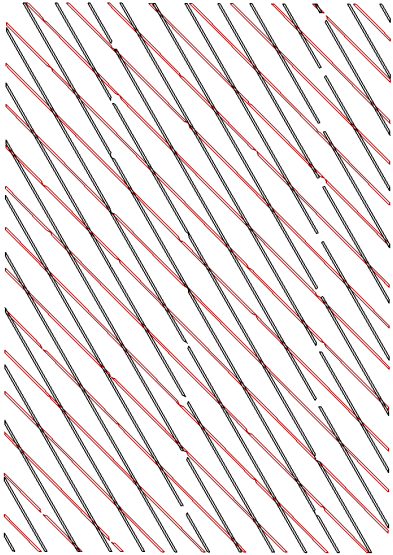
Gas mixing in two packing elements

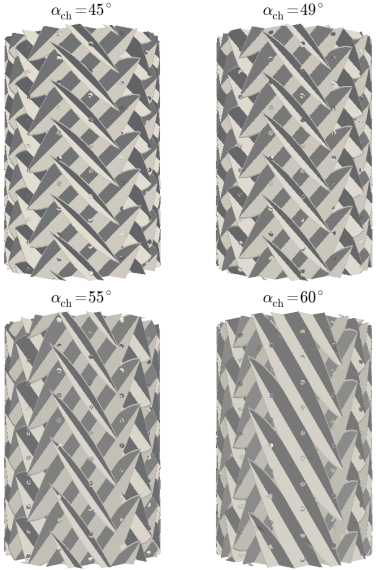
Seed: $\sigma_2 = \{(x, y, z) \in \mathcal{S} : x = -0.22\text{m}, 0.07^2\text{m} \leq y^2 + z^2 \leq 0.075^2\text{m}\}$



Single phase model – changes in the geometry

Different channel inclination angles and perforation densities





Single phase model – dry pressure loss estimation

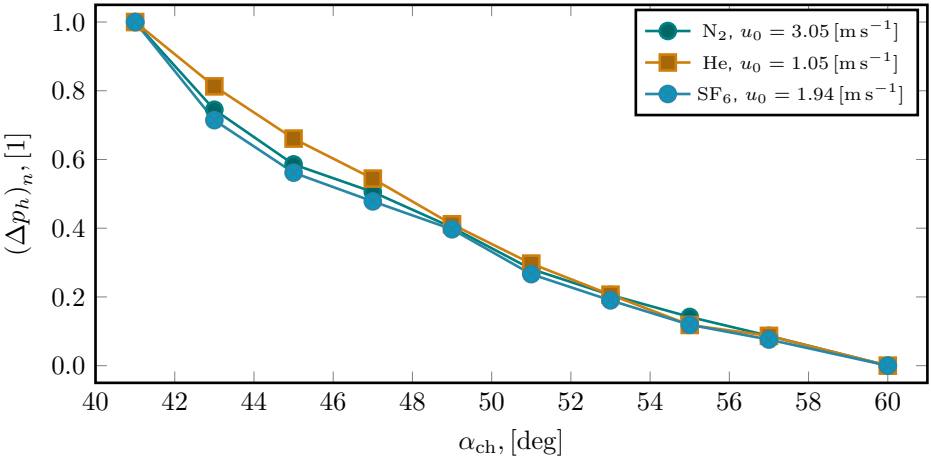
Different channel inclination angles

Variable for comparison: Normalized dry pressure loss

$$(\Delta p_h)_n^i := \frac{\Delta p_h^i - \min_{(i)} \Delta p_h}{\max_{(i)} \Delta p_h - \min_{(i)} \Delta p_h} \quad \in \langle 0, 1 \rangle$$

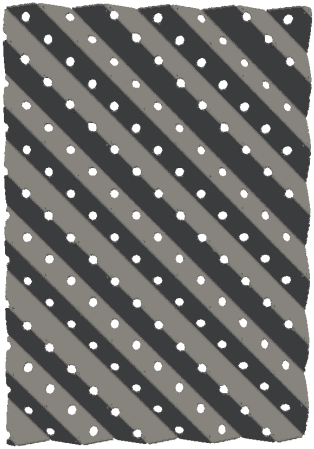
Single phase model – dry pressure loss estimation

Different channel inclination angles

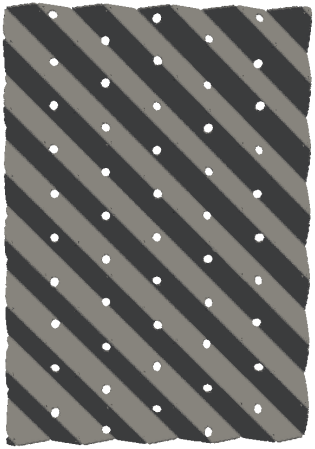


Single phase model – dry pressure loss estimation

Different perforation density



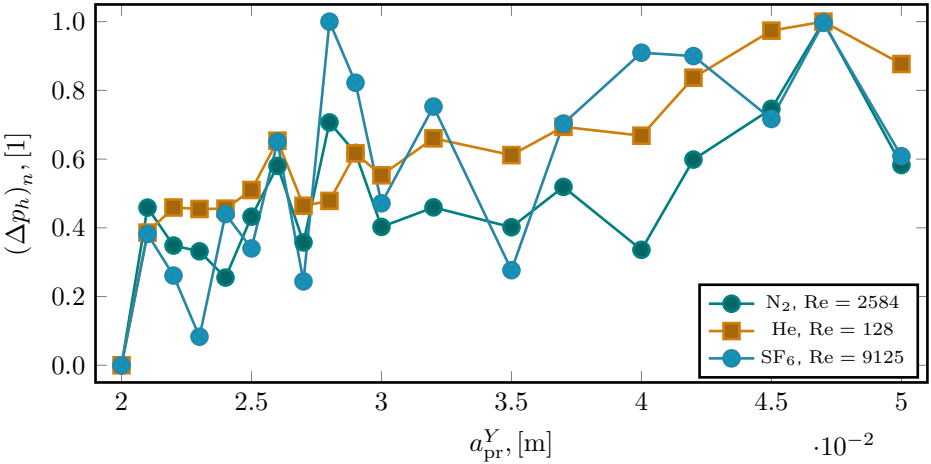
$$a_{\mathrm{pr}}^{Y} = 2.0 \cdot 10^{-2} \ \mathrm{m}$$



$$a_{\mathrm{pr}}^{Y} = 4.0 \cdot 10^{-2} \ \mathrm{m}$$

Single phase model – dry pressure loss estimation

Different perforation density



Single phase model – dry pressure loss estimation

Different perforation density

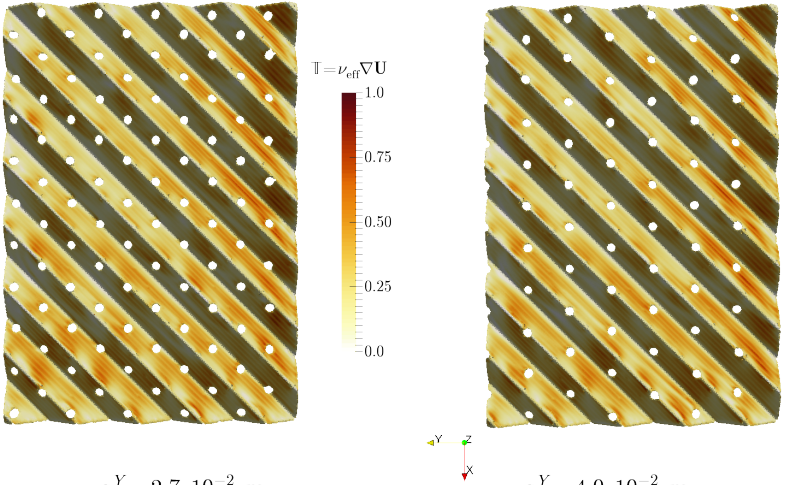
Ranges of Δp_h during the simulations

Case	Varied parameter	$\min \Delta p_h$, $\mathrm{Pa\,m^{-1}}$	$\max \Delta p_h$, $\mathrm{Pa\,m^{-1}}$
N_2	α_{ch}	112.96	439.00
He	α_{ch}	9.00	17.22
SF_6	α_{ch}	172.62	824.03
N_2	a_{pr}^{Y}	295.34	310.07
He	a_{pr}^{Y}	14.19	14.46
SF_6	a_{pr}^{Y}	530.16	543.85

- Channel inclination has substantially larger effect on Δp_h than perforation

Theory: Flow perturbation in the perforation vicinity

Wall shear stress on the packing

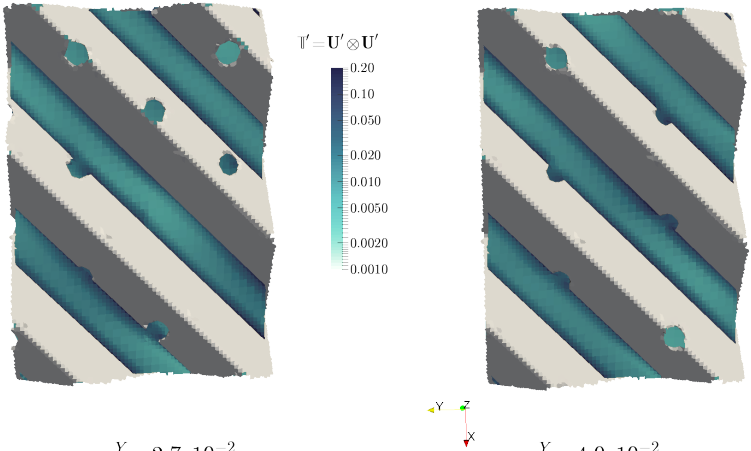


$a_{\mathrm{pr}}^{Y} = 2.7 \cdot 10^{-2}$ m

$a_{\mathrm{pr}}^{Y} = 4.0 \cdot 10^{-2}$ m

Theory: Flow perturbation in the perforation vicinity

Reynolds stress around holes



$a_{\mathrm{pr}}^{Y} = 2.7 \cdot 10^{-2}$ m

$a_{\mathrm{pr}}^{Y} = 4.0 \cdot 10^{-2}$ m