CFD study of gas flow through structured separation columns packings Mellapak 250.X and Mellapak 250.Y

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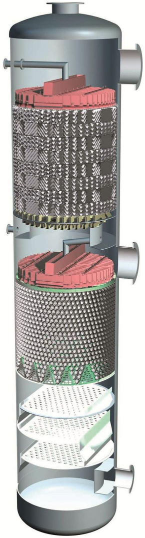
Introduction

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 $\rightarrow$ non-steady process
- Complex geometry
- Simultaneous heat and mass transfer

Separation columns modeling

Multiphase flow, simultanous heat and mass transfer

Mass and momentum balance, N phases

$$\begin{aligned}\rho_i \frac{\partial}{\partial t}(\mathbf{U}_i) + \nabla \cdot (\rho_i \mathbf{U}_i \otimes \mathbf{U}_i) &= \nabla \cdot \tau + F_i, \quad i = 1, \ldots, N \\ \rho_i = \rho(c_i, T_i), \quad \nabla \cdot (\mathbf{U}_i) &= S_i^{\rho} = \sum_{j=1}^{M} \hat{R}_{i,j}^{c}\end{aligned}$$

Mass transfer, M species

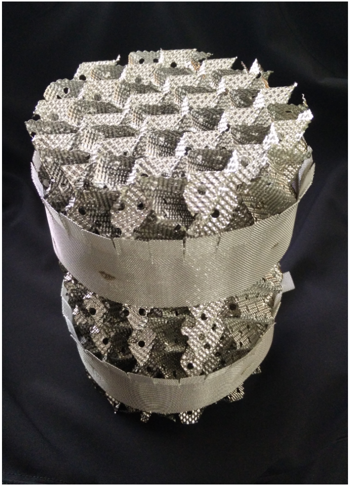
$$\frac{\partial}{\partial t} c_{i,j} + \nabla \cdot (\mathbf{U}_i \, c_{i,j}) = \nabla \cdot \left(\Gamma_{i,j}^{c} \, \nabla c_{i,j} \right) + S_{i,j}^{c}, \qquad j = 1, \ldots, M$$

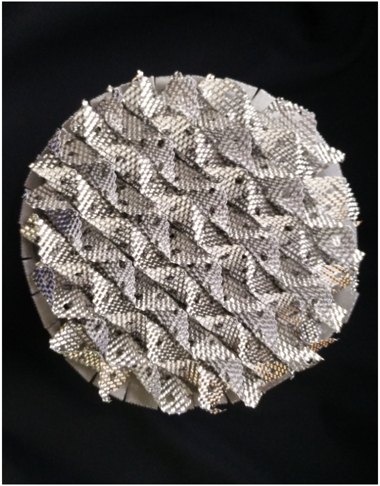
Heat transfer, N phases

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

Mellapak type structured packing

Corrugated, perforated sheet of steel equipped with texture

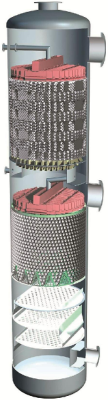




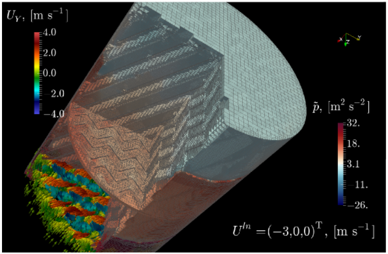
Possible simplifications

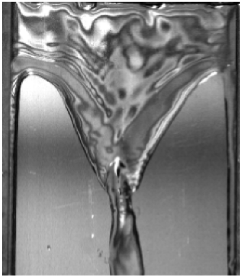
Approach the problem from two different sides

keep geometry,
simplify flow



simplify geometry,
keep flow



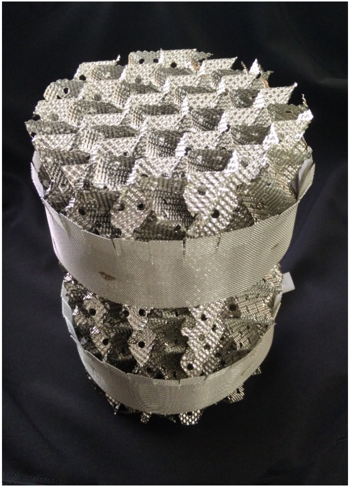


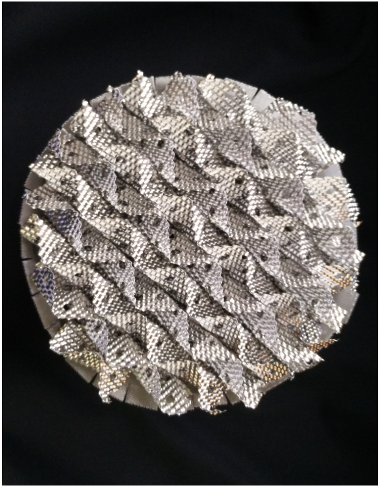
Applied model

Problem geometry

Mellapak 250.X & Mellapak 250.Y, 1 or 2 packing elements

Selected approach: Keep geometry, simplify flow

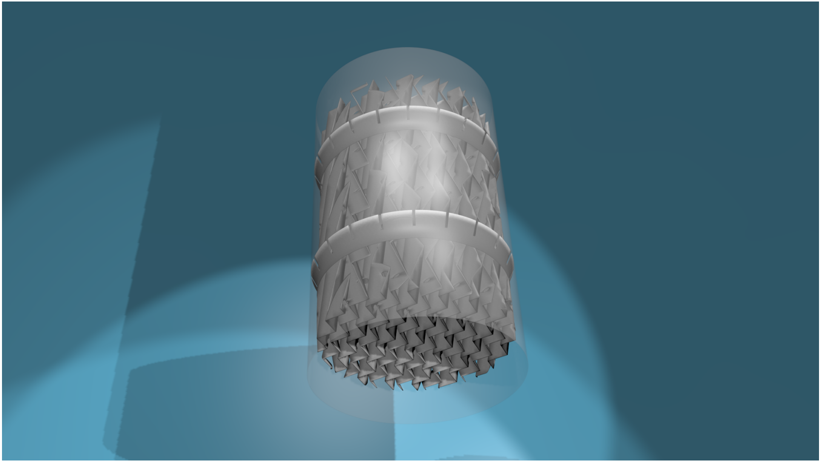




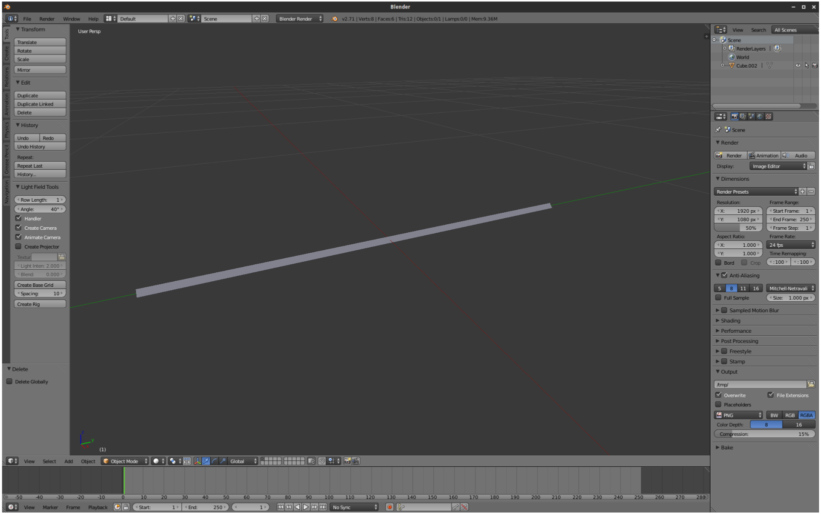
Problem geometry

Mellapak 250.X & Mellapak 250.Y, 1 or 2 packing elements

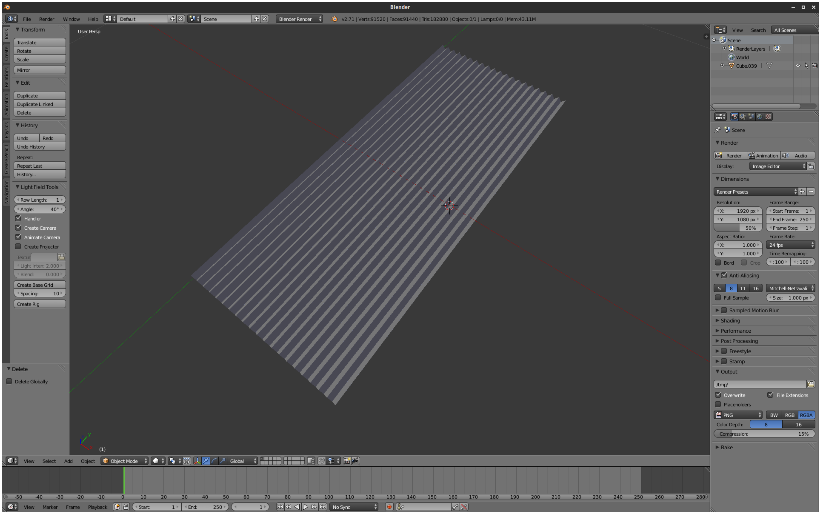
Geometry example: Mellapak 250.X



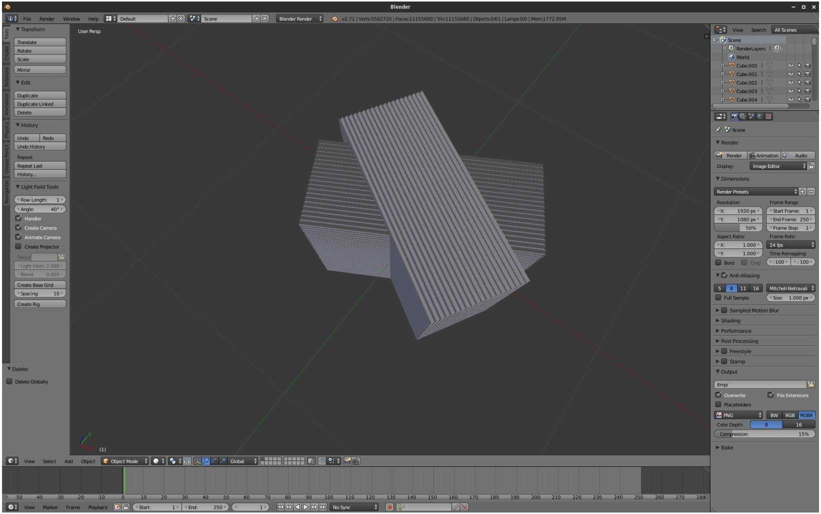
Step 1: Create base packing element



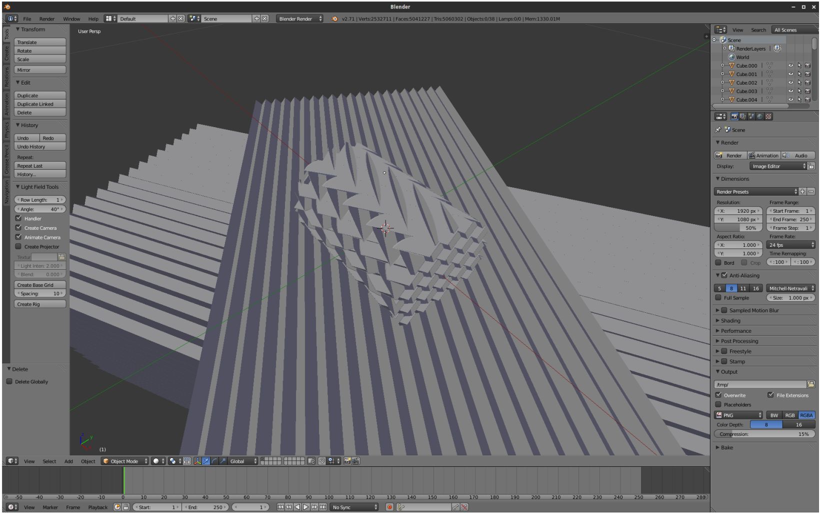
Step 2: Construct one corrugate sheet



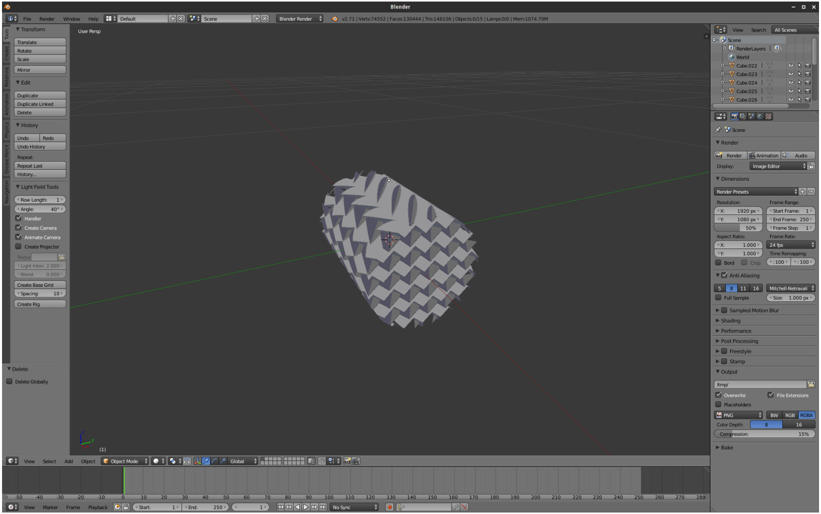
Step 3: Prepare all the needed sheet



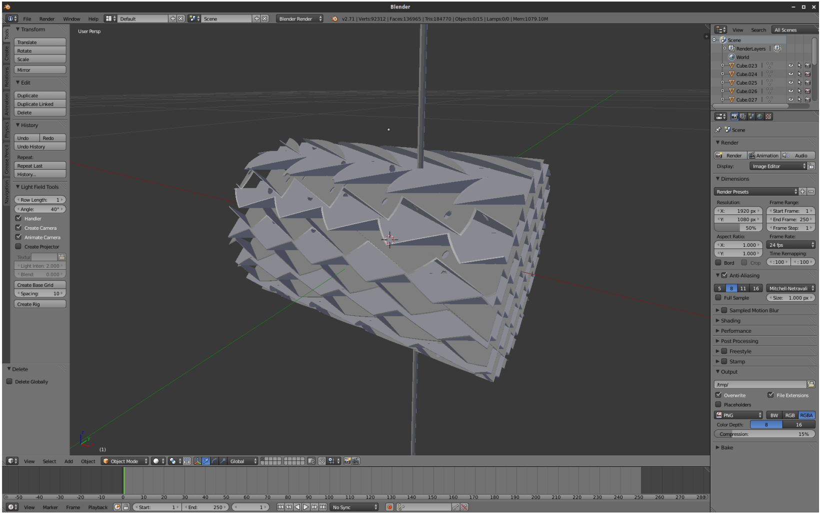
Step 4: Cut out the desired packing shape



Step 4: Cut out the desired packing shape



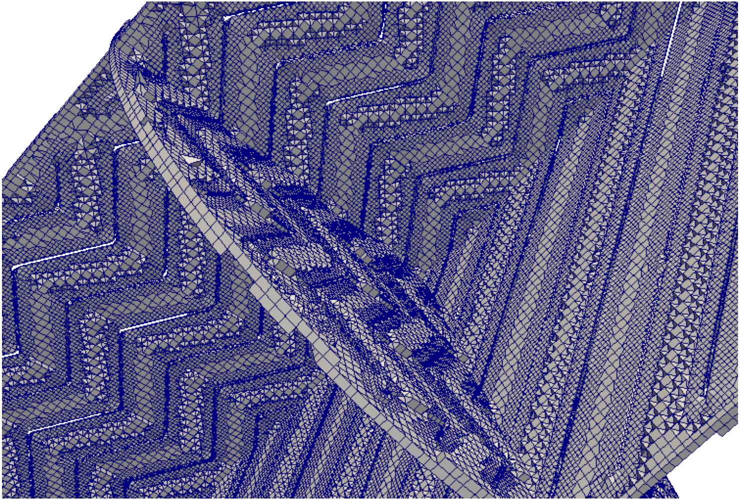
Step 5: Perforate the packing



Step 6: Finish the packed bed generation

Geometry meshing
OpenFOAM core tool for FVM meshes generation – snappyHexMesh

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



Model equations

RANS + SST $k - \omega$

Navier-Stokes equations

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

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

SST $k - \omega$ model

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

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

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

BC

$$\mathbf{U} = G(\mathbf{U})$$

$$\tilde{p} = H(p)$$

$$k = K(k)$$

$$\omega = L(\omega)$$

on $\partial \Omega^h$

IG

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

in Ω^h

Closer look on boundary conditions

The used mesh is fine enough to omit wall functions

$\mathcal{S}_{\text{inlet}} = \{(x,y,z) \in \mathbb{R}^3 : x = h_{\text{col}}, y^2 + z^2 \leq r_{\text{col}}^2\}$

$$\mathbf{U} = (-u_i, 0, 0)^{\mathrm{T}}, \quad \mathbf{S}_f \cdot \nabla p = 0, \quad k = k_0, \quad \omega = \omega_0$$

$\mathcal{S}_{\text{outlet}} = \{(x,y,z) \in \mathbb{R}^3 : x = -h_{\text{col}}, y^2 + z^2 \leq r_{\text{col}}^2\}$

$$\mathbf{S}_f \cdot \nabla \mathbf{U} = (0,0,0)^{\mathrm{T}} \text{ if } \mathbf{\Phi} > 0,\ \mathbf{U} = (0,0,0)^{\mathrm{T}} \text{ else}$$

$$p = 0$$

$$\mathbf{S}_f \cdot \nabla k = 0 \text{ if } \mathbf{\Phi} > 0,\ k = k_0 \text{ else}, \quad \mathbf{S}_f \cdot \nabla \omega = 0 \text{ if } \mathbf{\Phi} > 0,\ \omega = \omega_0 \text{ else}$$

$$\mathbf{\Phi} = \mathbf{S}_f \cdot \mathbf{U}$$

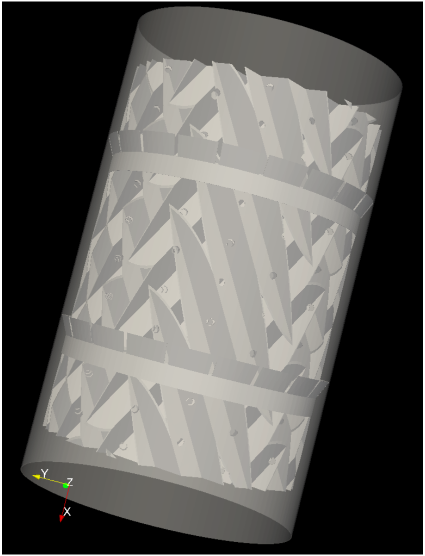
$\mathcal{S}_{\text{wall}} = B \cup \{(x,y,z) \in \mathbb{R}^3 : x = \langle -h_{\text{col}}, -h_{\text{col}} \rangle, y^2 + z^2 = r_{\text{col}}^2\}$

$$\mathbf{U} = (0,0,0)^{\mathrm{T}}, \quad \mathbf{S}_f \cdot \nabla p = 0, \quad \mathbf{S}_f \cdot \nabla k = 0, \quad \mathbf{S}_f \cdot \nabla \omega = 0$$

Results

Measurable variable

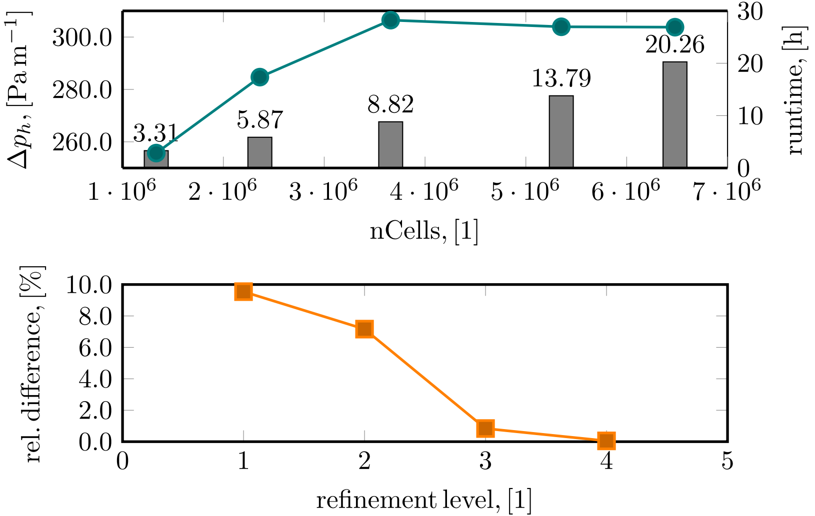
Due to the apparatus complexity, there is not much to be measured



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

Mesh size determination

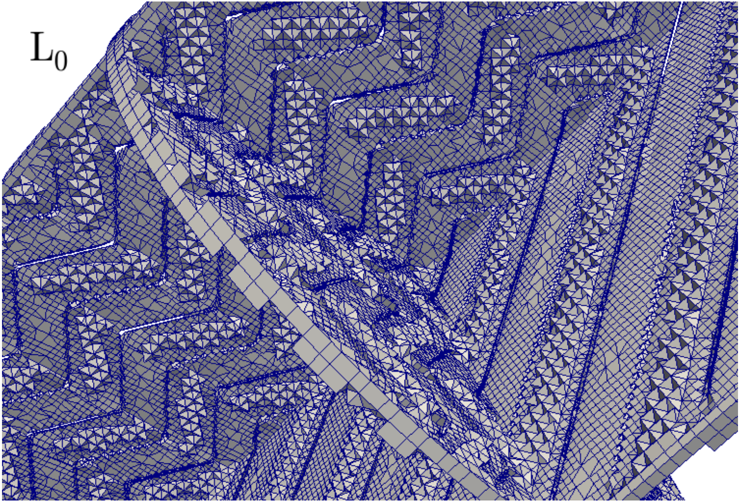
Main variable of interest is dry pressure loss, Δp_h



Mesh size determination

Main variable of interest is dry pressure loss, Δp_h

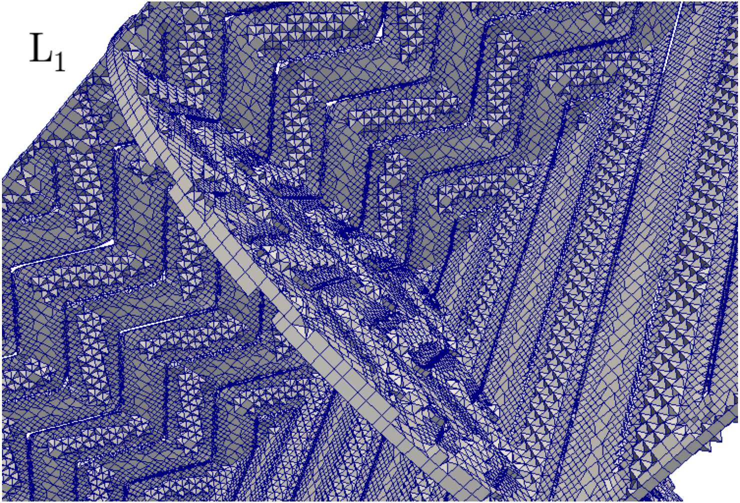
Mesh sizes: Mesh with $\mathrm{nCells} \approx 1 \cdot 10^6$/packing element



Mesh size determination

Main variable of interest is dry pressure loss, Δp_h

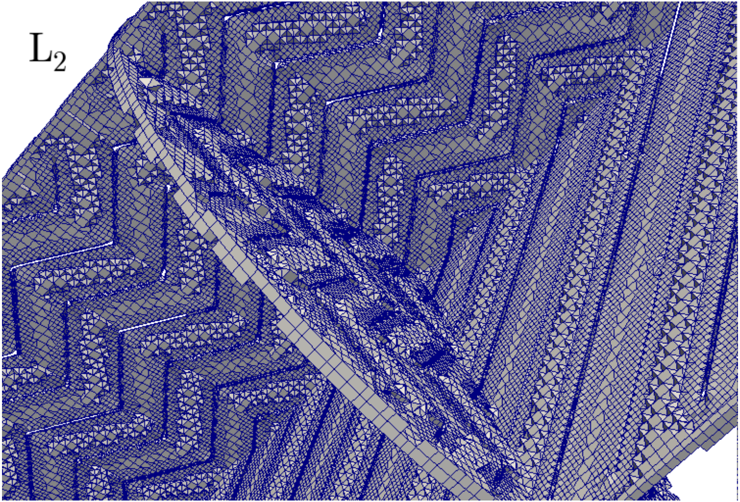
Mesh sizes: Mesh with $\mathrm{nCells} \approx 2.5 \cdot 10^6$/packing element



Mesh size determination

Main variable of interest is dry pressure loss, Δp_h

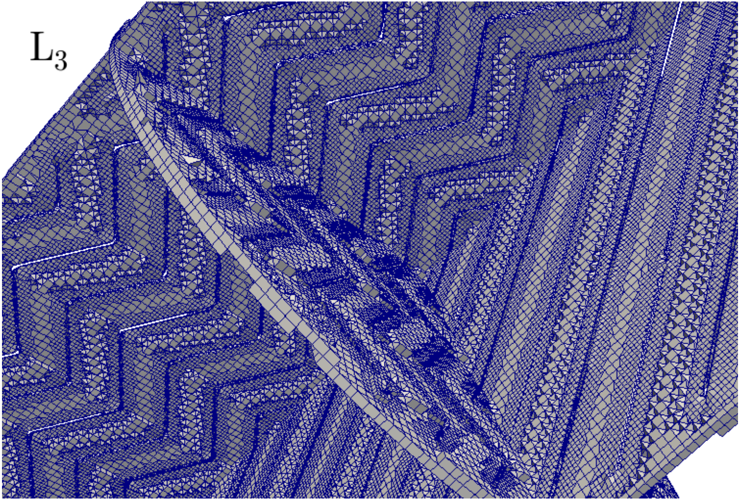
Mesh sizes: Mesh with $\mathrm{nCells} \approx 3.8 \cdot 10^6$/packing element



Mesh size determination

Main variable of interest is dry pressure loss, Δp_h

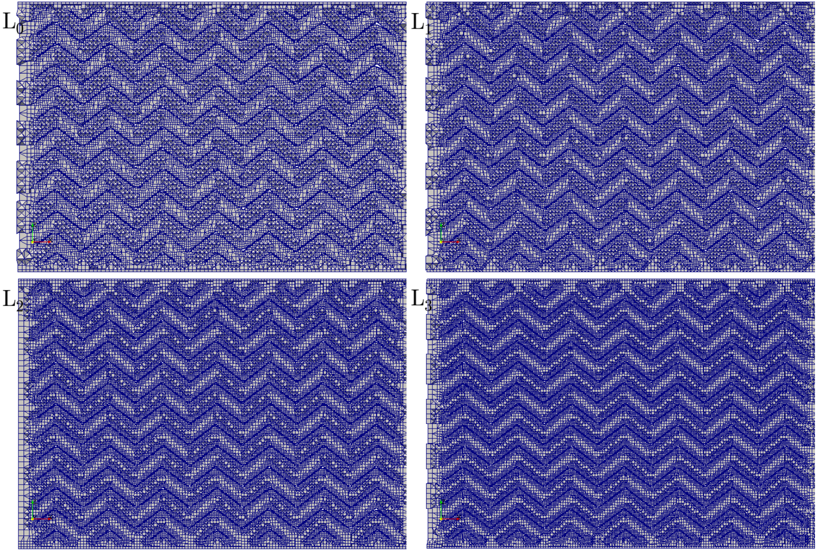
Mesh sizes: Mesh with $\mathrm{nCells} \approx 5.3 \cdot 10^6$/packing element



Mesh size determination

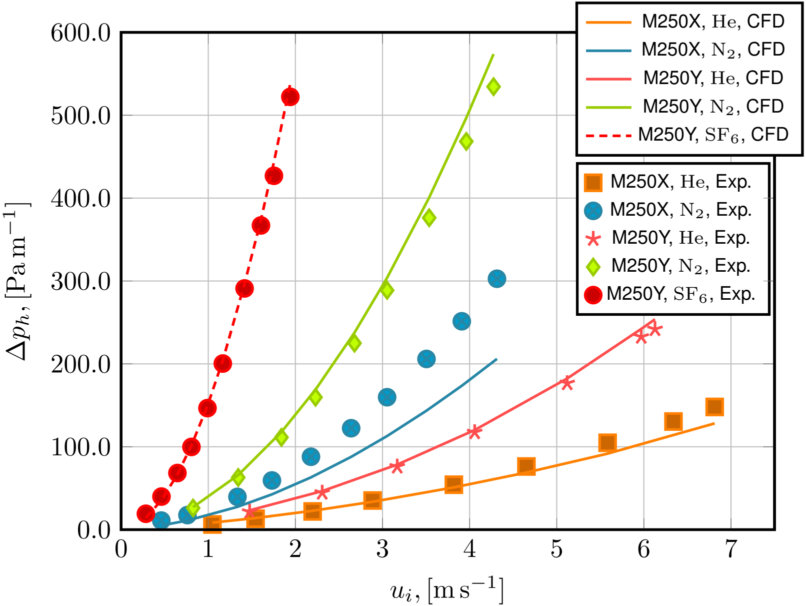
Main variable of interest is dry pressure loss, Δp_h

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



Model validation on experimental data

Data measured by Mass Transfer Laboratory at UCT Prague



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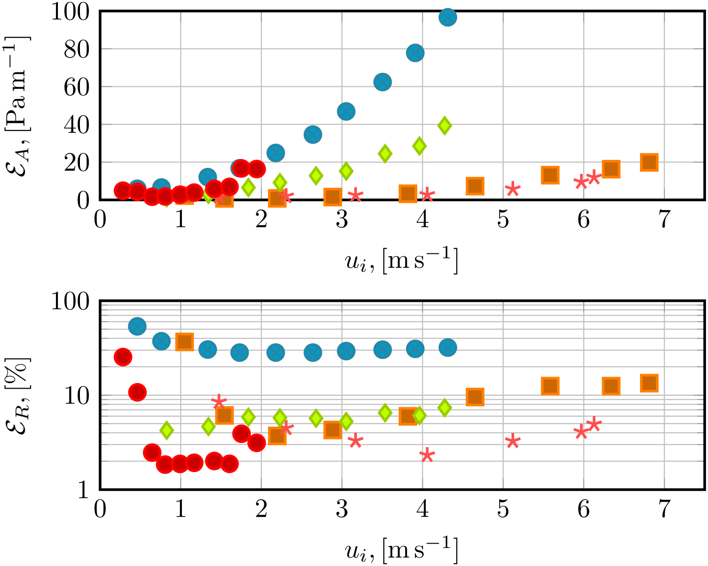
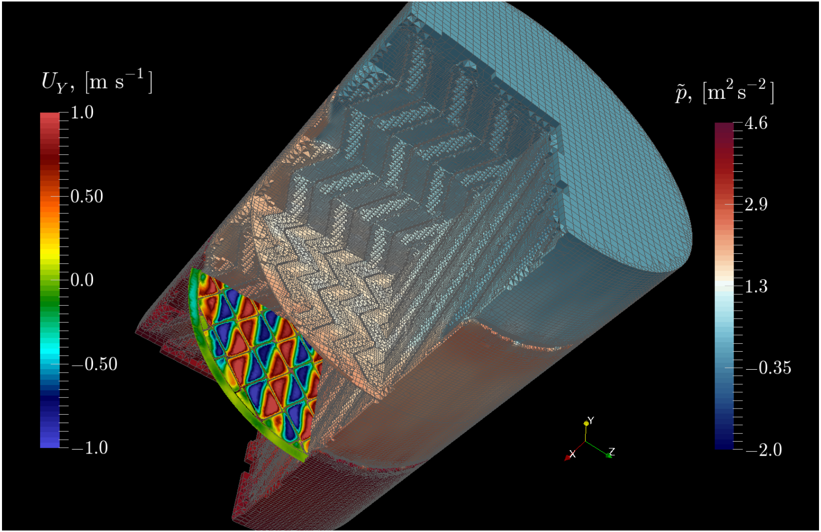
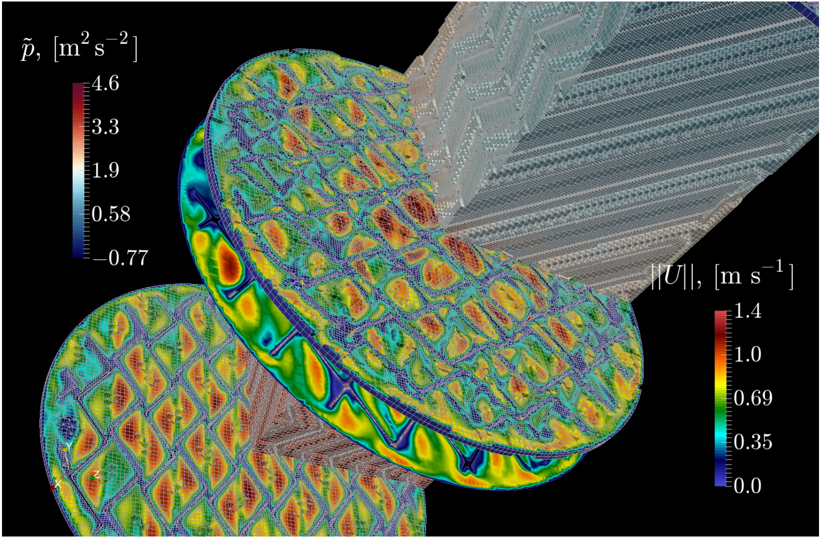


Result: flow patterns in 1 packing packing element



Flow in two packing elements

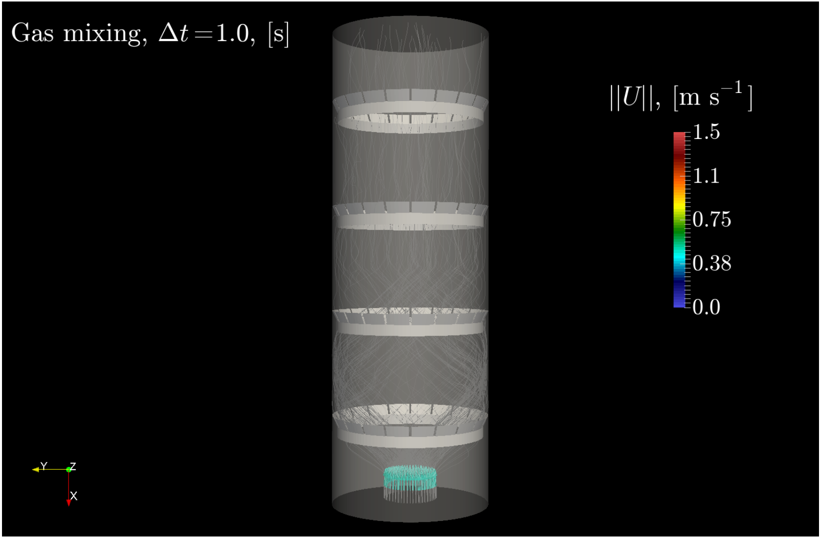
Simulation: Change of flow at transition between packing elements



Mellapak packing mixing properties

Gas mixing in two packing elements

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



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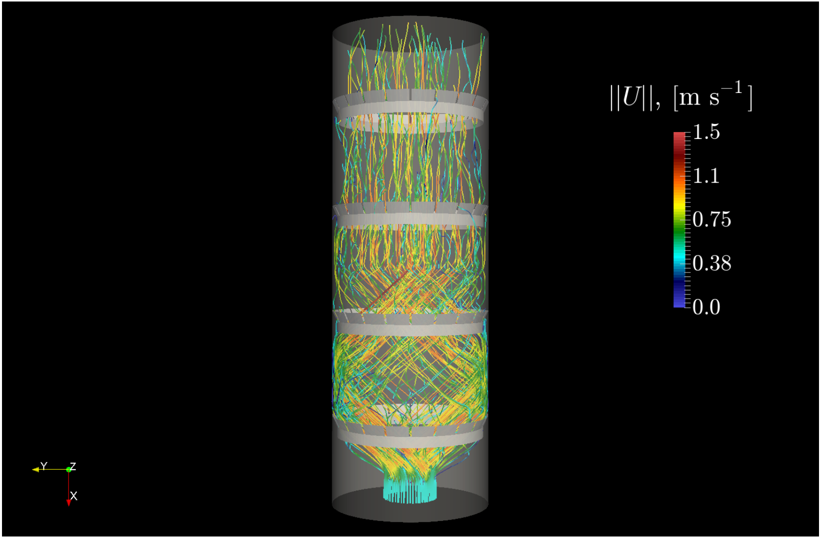
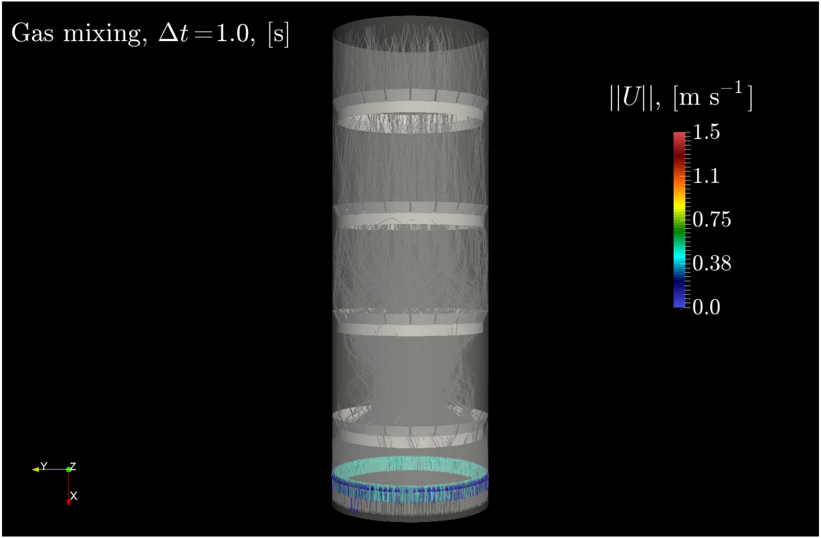


Mellapak packing mixing properties

Gas mixing in two packing elements

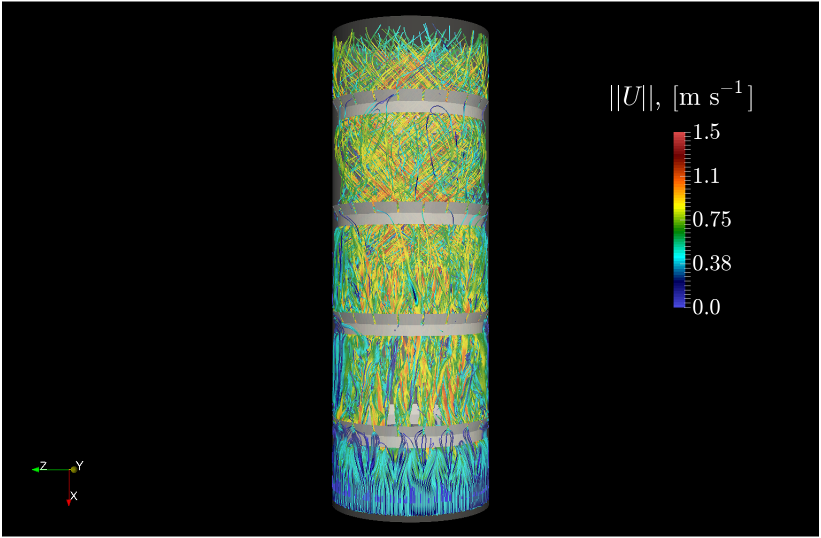
Seed: $\sigma_2 = \{(x, y, z) \in \mathcal{S} : x = -0.22\text{m}, 0.07^2\text{m} \leq y^2 + z^2 \leq 0.075^2\text{m}\}$



Mellapak packing mixing properties

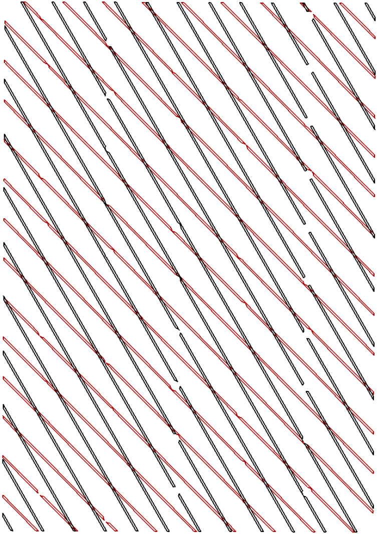
Gas mixing in two packing elements

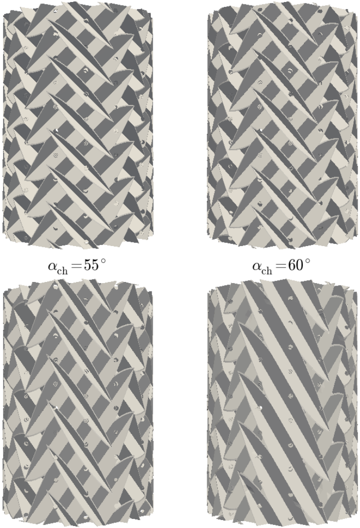
Seed: $\sigma_2 = \{(x,y,z) \in \mathcal{S} : x = -0.22\text{m}, 0.07^2\text{m} \leq y^2 + z^2 \leq 0.075^2\text{m}\}$



Changes in the geometry

Different channel inclination angles and perforation densities



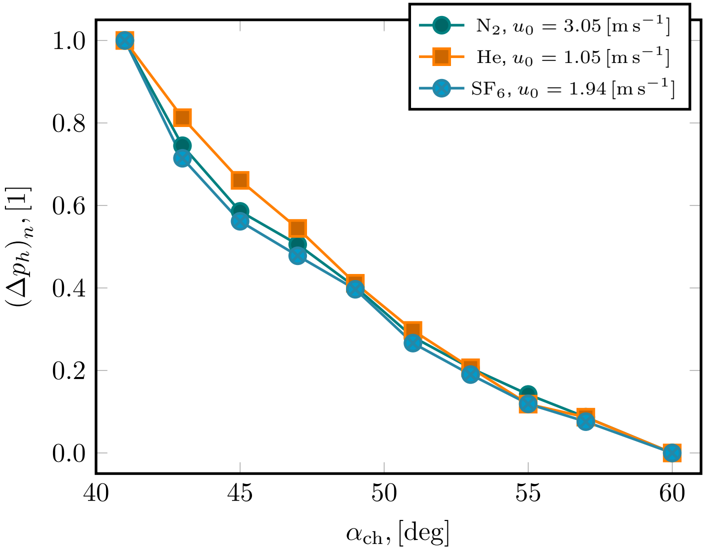


Variable for comparison: Normalized dry pressure loss

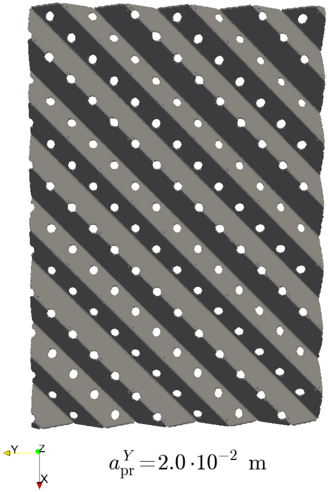
$$(\Delta p_h)_n^i := \frac{\Delta p_h^i - \min_{(i)} \Delta p_h}{\max_{(i)} \Delta p_h - \min_{(i)} \Delta p_h} \quad \in \langle 0, 1 \rangle$$

Dry pressure loss estimation

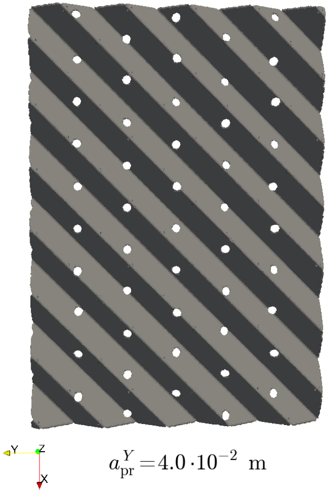
Different channel inclination angles



Dry pressure loss estimation
Different perforation density



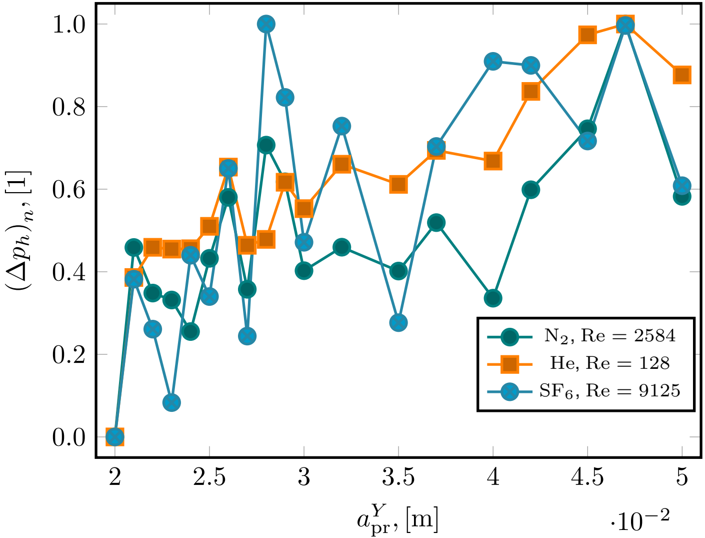
$a_{\text{pr}}^{Y} = 2.0 \cdot 10^{-2}\ \text{m}$



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

Dry pressure loss estimation

Different perforation density



Dry pressure loss estimation

Different perforation density

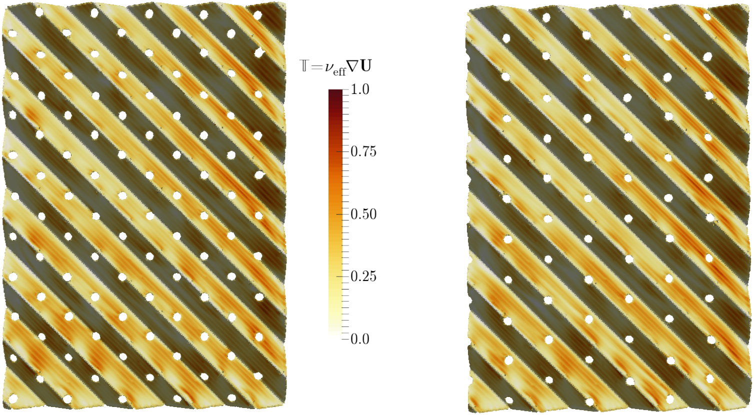
Ranges of Δp_h during the simulations

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

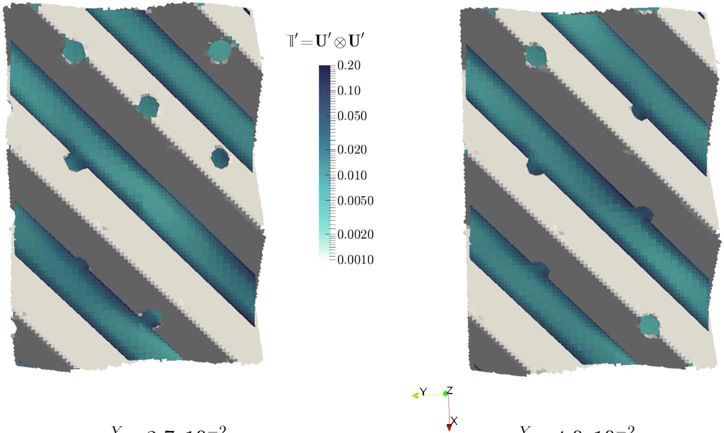


$a_{\text{pr}}^{Y} = 2.7 \cdot 10^{-2}$ m

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

Theory: Flow perturbation in the perforation vicinity

Reynolds stress around holes



$a^Y_{\mathrm{pr}} = 2.7 \cdot 10^{-2}$ m

$a^Y_{\mathrm{pr}} = 4.0 \cdot 10^{-2}$ m

Conclusions

Prepared:

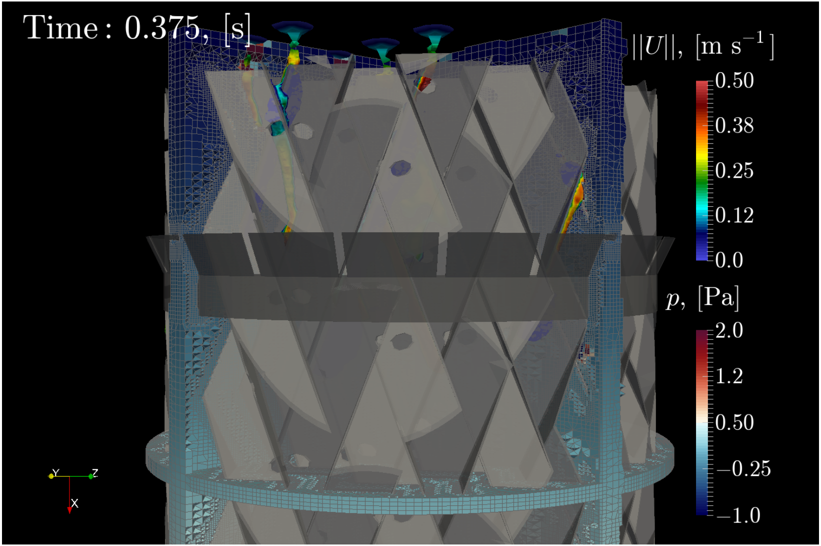
- Algorithm for automatic geometry generation
- Automatized case construction and solution
- Tools for dry pressure loss estimation based on flow and geometry parameters.

To do:

- Axial dispersion in the gas phase
- Different types of structured packings
- Multiphase flows

Next steps

Simulations of multiphase flow in Mellapak type packings, cooperation with IT4I



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References

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Thank you for your attention