Flow and deposition simulation related to chromatographic separation processes

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12th European Congress for Stereology and Image Analysis
11. – 14. September 2017
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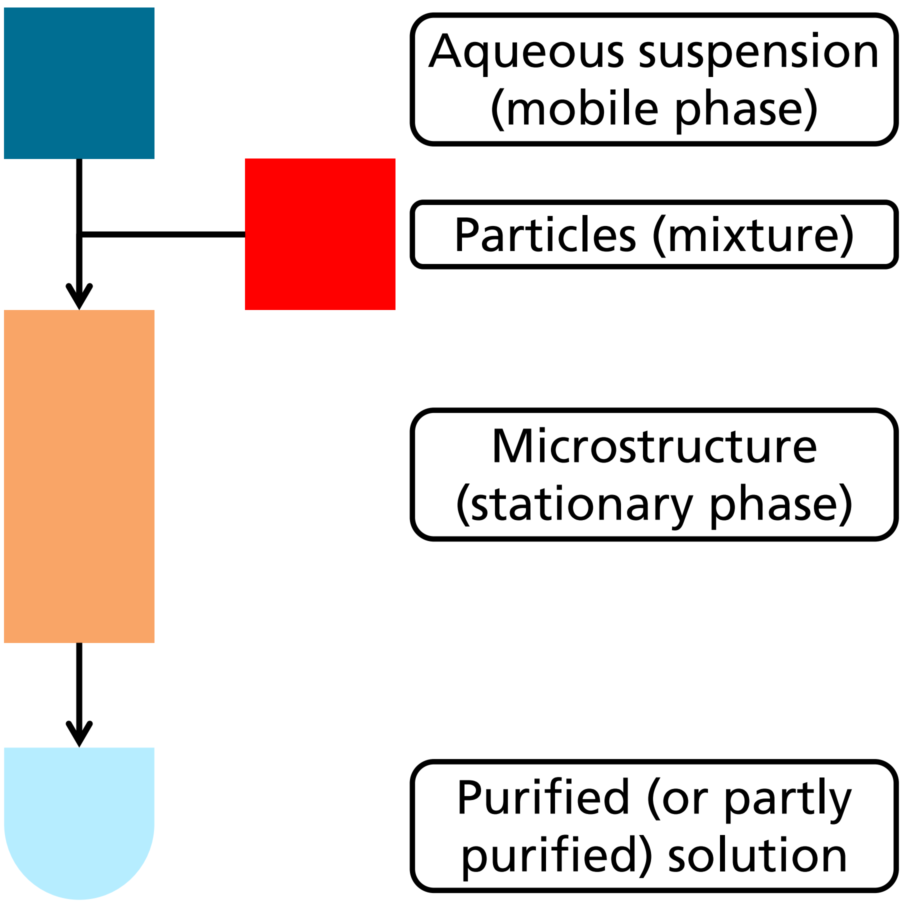
Chromatography



Examples:

- Separation of cancerous from healthy cells
- Separation of blood cells from blood plasma
- Separation of proteins from solutions

Outline

- Fluid dynamics
  - Flow simulation
  - Particle motion
- Microstructures
  - Foam structure
  - Fiber structure
  - Deterministic lateral device (DLD)
- Results
- Summary and conclusions

Goal: Identify characteristics of porous medium influencing filtration properties

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Flow

- Describe flow through a porous medium by velocity field u and pressure distribution p
- Assume slow and incompressible viscous flow (stationary Stokes equations)

$$\begin{aligned} \nabla \cdot u &= 0, \\ -\mu \Delta u &= -\nabla p + f, \end{aligned}$$

  where f denotes external body forces and μ the fluid viscosity
- Consider representative volume element (periodic in x and y-direction)
- Boundary conditions
  - x and y-direction: periodic
  - z-direction: periodic (with given mean velocity)
  - Wall: no slip

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Particle motion

- Describe motion of a single particle

$$\frac{dx}{dt} = v$$
$$\frac{dv}{dt} = \gamma(v-u) + \sigma\frac{dW(t)}{dt} + q\frac{E}{m}$$

where v is the velocity of the particle

x	Particle position	dW	3d probability measure
v	Particle velocity	q	Particle charge
γ	Friction coefficient	E	Electric field
σ	fluctuation-dissipation term	m	Particle mass

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Particle motion (cont.)

- Particles are considered as
  - Spherical
  - Solid
- Deposition model sieving
  - Particles are considered as caught, if they don‘t move any more

    -> particle lie on two (or more) different points of the structure

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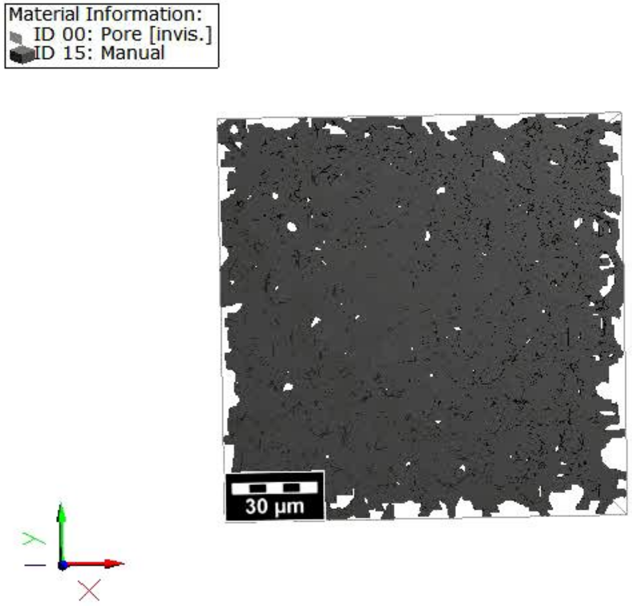
Foam structures

- Foam is reproduced from µCT-images (Liebscher et al. 2015)
- Model is based on Laguerre tessellation
- Model is fitted to the properties of the real foam structure
  - Cell volume, surface area, …
  - Fitting is a two step procedure
- Size of microstructure

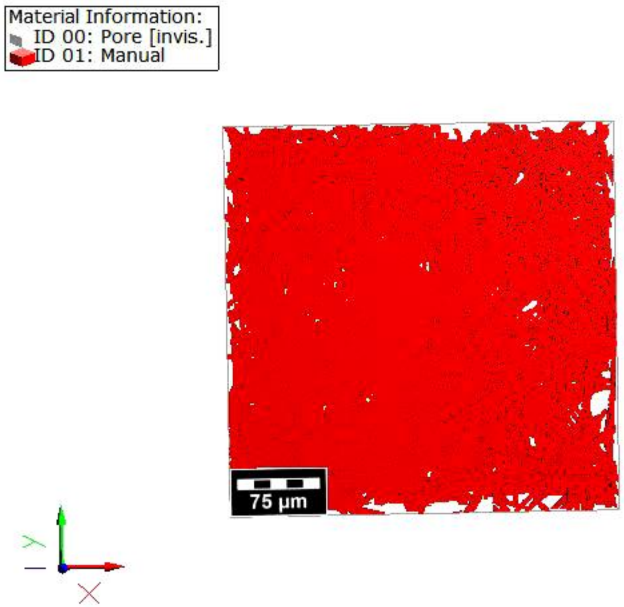
  $656 \times 656 \times 656$ voxels
- Porosity $\sim 87.5\ \%$



Liebscher et al., Modelling of open cell foams based on 3D image data, 20th International conference on composite materials, 2015

Fiber structure

- Fibrous medium is simulated matching to SEM images
- Fibers are modeled as chain of spheres (Easwaran et al. 2016)
- Anisotropic structure
- Size of microstructure
  $750 \times 750 \times 512$ voxels
- Porosity $\sim 89.5\ \%$
- Fiber diameter $10\ \mu m$
  (voxel size $1\ \mu m$)

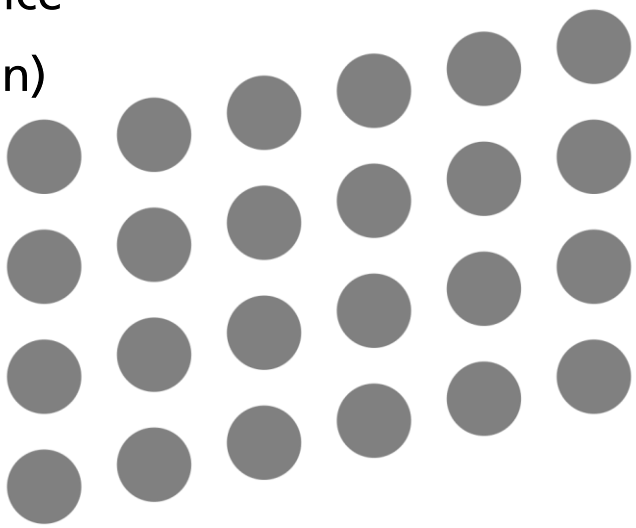


Easwaran et al., Automatic fiber thickness measurement in scanning electron microscopy images validated using synthetic data, Chem. Eng. Technol., 39(3), 395-402, 2016

Deterministic lateral device (DLD)

- Use specific arrangement of posts within a channel
- Lateral shift of posts in succeeding columns
- Control trajectories of different sized particles
- Separation of particles smaller and larger as a critical diameter

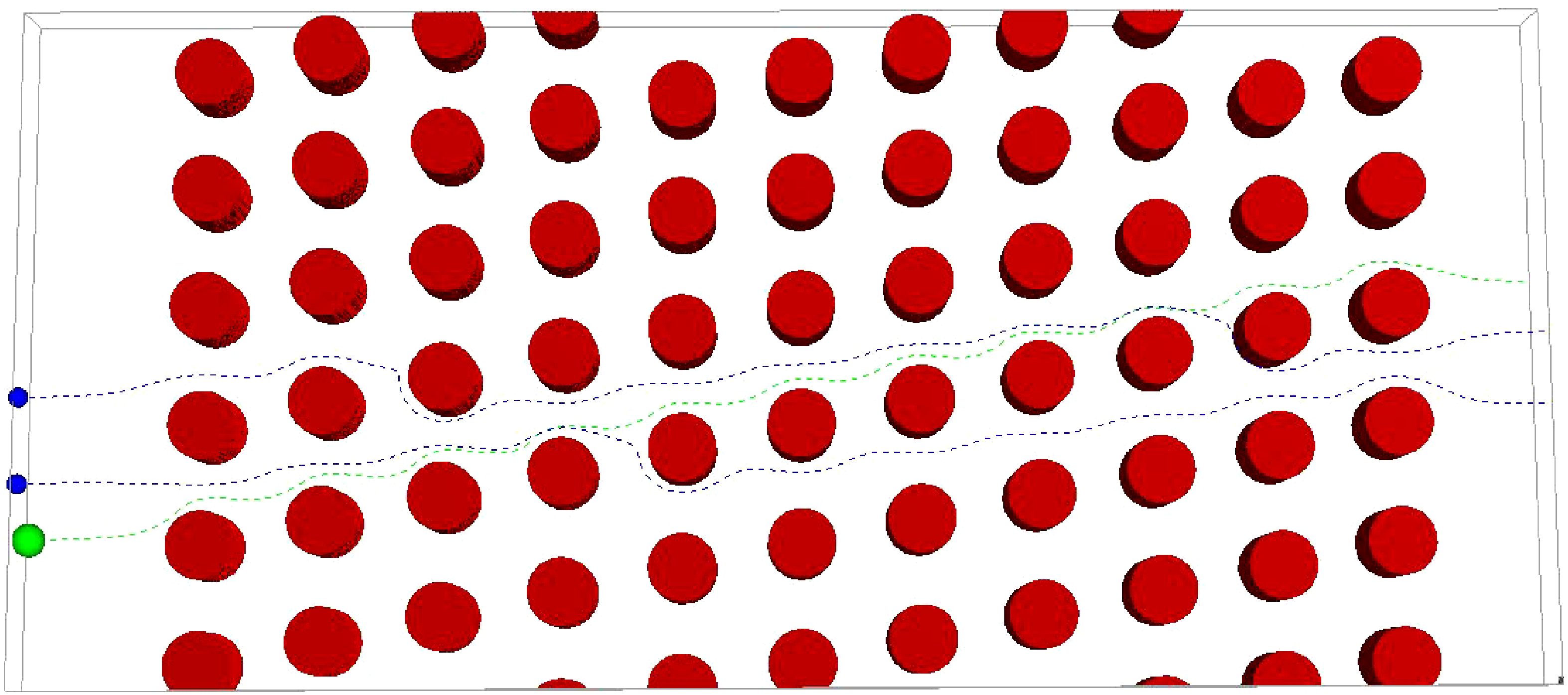
  -> different escape height in the device
- 100% separation efficiency (by design)



Example
- Periodicity 5
- Gap size equal in x and y direction
- Deflection $11.31°$

J. McGrath et al.(2014), Deterministic lateral displacement for particle separation: a review

DLD – cont.



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Results

Basic settings

- Simulate flow and particle motion
- Fluid: water
- Flow velocity $0.001\ m/s$
- Two different particle sizes: $6\ \mu m$ and $10\ \mu m$
- Use commercial software GeoDict

Modeling of foam and fibrous structure

- Try to achieve 100% separation efficiency as for the DLD device
- Duplicate REV in depth direction and choose suitable structure size
- Identify suitable criteria

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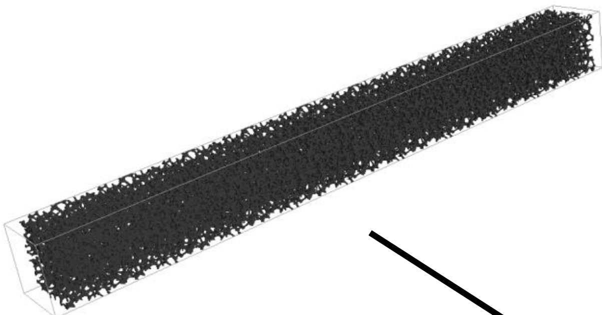
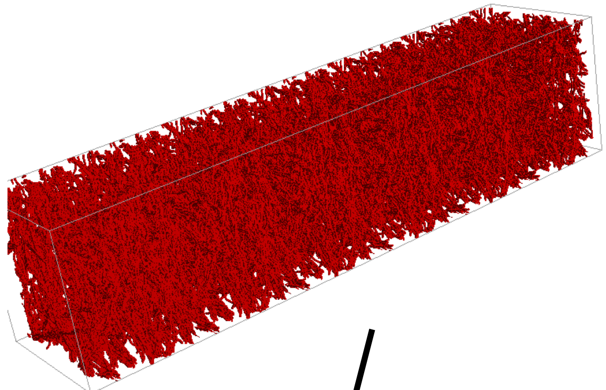
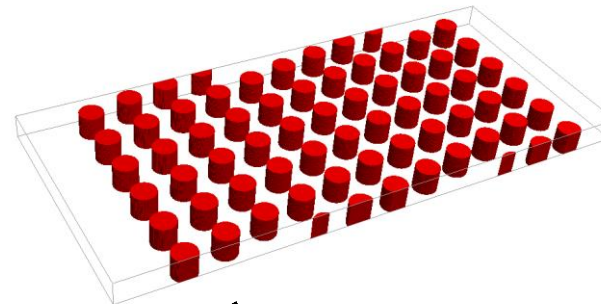
Results – Setup



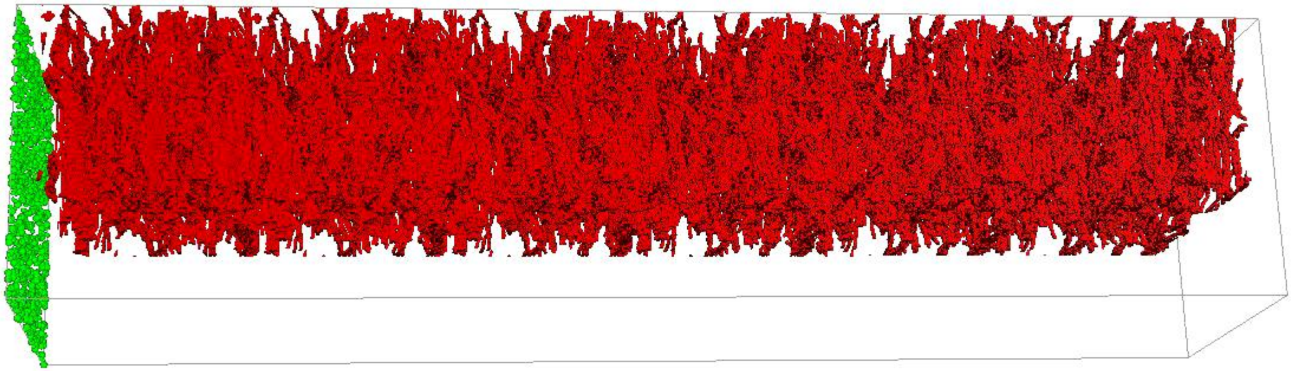




Pressure drop Δp (difference between inlet and outlet)

Efficiency $E = 1 - \frac{\#particles\ outlet}{\#particles\ inlet}$

Fluid flow



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Results – Foam

- Use 3 different realizations of the same stochastic model (REV)
  - Porosity $\sim 87.5\%$ (independent of structure size and thickness)
- Rescale the size of structure and duplicate in z-direction

-> $164\ \mu m$, ($0.25\ \mu m$ voxel) $328\ \mu m$ ($0.5\ \mu m$ voxel)

-> duplicate to thickness $1640\ \mu m$

Voxel size	$\mathbf{0.25\ \mu m}$	$\mathbf{0.5 \mu m}$
Duplication	10x	5x
Average pore size	$26\ \mu m$	$52.8\ \mu m$
Estimated surface area	$3.8 \cdot 10^{-6} m^2$	$8.0 \cdot 10^{-6} m^2$

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Results – Foam (cont.)

- Results in terms of pressure drop and filter efficiency
- Duration of $1000\ s$

Voxel size	$\mathbf{0.25\ \mu m}$	$\mathbf{0.5\ \mu m}$
Initial pressure drop	$154\ Pa$	$40\ Pa$
Pressure drop ($1000\ s$)	$157\ Pa$	$41\ Pa$
Initial efficiency ($10\ \mu m$)	$92\ \%$	$21\ \%$
Final efficiency ($10\ \mu m$)	$97\ \%$	$18\ \%$
Initial efficiency ($6\ \mu m$)	$22\ \%$	$4\ \%$
Final efficiency ($6\ \mu m$)	$43\ \%$	$4\ \%$

Results – Fiber structure

- Use 3 different realizations of the same stochastic model (REV)
  - Porosity $\sim 89.5\%$ (independent of structure size and thickness)
- Rescale the size of structure and duplicate in z-direction

-> $256\ \mu m$ ($0.5\ \mu m$ voxel), $512\ \mu m$ ($1 \mu m$ voxel)

-> duplicate to thickness $1536\ \mu m$

Voxel size	$\mathbf{0.5}\ \boldsymbol{\mu m}$	$1\ \boldsymbol{\mu m}$
Duplication	6x	3x
Average pore size	$33\ \mu m$	$65\ \mu m$
Estimated surface area	$2.3 \cdot 10^{-5} m^2$	$3.6 \cdot 10^{-5} m^2$

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Results – Fiber structure (cont.)

- Results in terms of pressure drop and filter efficiency
- Duration of $1000\ s$

Voxel size	$\mathbf{0.5\ \mu m}$	$\mathbf{1\ \mu m}$
Initial pressure drop	$62\ Pa$	$15\ Pa$
Pressure drop ($1000\ s$)	$64\ Pa$	$16\ Pa$
Initial efficiency ($10\ \mu m$)	$98\ \%$	$30\ \%$
Final efficiency ($10\ \mu m$)	$96\ \%$	$26\ \%$
Initial efficiency ($6\ \mu m$)	$62\ \%$	$12\ \%$
Final efficiency ($6\ \mu m$)	$62\ \%$	$14\ \%$

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Results – Foam

- To increase the internal surface dilate the structure (enlarge thickness of struts)

	Foam (5x 328 μm)		
Dilation	$0\ \mu m$	$1\ \mu m$	$2\ \mu m$
Porosity	0.875	0.8383	0.7889
Est. surface area	$8.0 \cdot 10^{-6} m^2$	$8.6 \cdot 10^{-6} m^2$	$9.5 \cdot 10^{-6} m^2$
Mean pore size	$52.8\ \mu m$	$51\ \mu m$	$49\ \mu m$
$\Delta p(0\ s)$	$40\ Pa$	$50\ Pa$	$69\ Pa$
$\Delta p(1000\ s)$	$41\ Pa$	$51\ Pa$	$69\ Pa$
$E(10\mu m, 0\ s)$	21 %	20 %	28 %
$E(10\ \mu m, 1000\ s)$	18 %	16 %	25 %
$E(6\ \mu m, 0\ s)$	4 %	5 %	6 %
$E(6\ \mu m, 1000\ s)$	4 %	6 %	6 %

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Results – Fiber structure

- To increase the internal surface dilate the structure (enlarge diameter of fibers)

	Fiber structure (3x 512 μm)		
Dilation	$0\ \mu m$	$1\ \mu m$	$2\ \mu m$
Porosity	0.895	0.86	0.825
Est. surface area	$3.6 \cdot 10^{-5} m^2$	$3.6 \cdot 10^{-5} m^2$	$3.55 \cdot 10^{-5} m^2$
Mean pore size	$65\ \mu m$	$63\ \mu m$	$61\ \mu m$
$\Delta p(0\ s)$	$15\ Pa$	$18\ Pa$	$21\ Pa$
$\Delta p(1000\ s)$	$16\ Pa$	$18\ Pa$	$21\ Pa$
$E(10\mu m, 0\ s)$	30 %	29 %	35 %
$E(10\ \mu m, 1000\ s)$	26 %	30 %	26 %
$E(6\ \mu m, 0\ s)$	12 %	11 %	11 %
$E(6\ \mu m, 1000\ s)$	14 %	13 %	11 %

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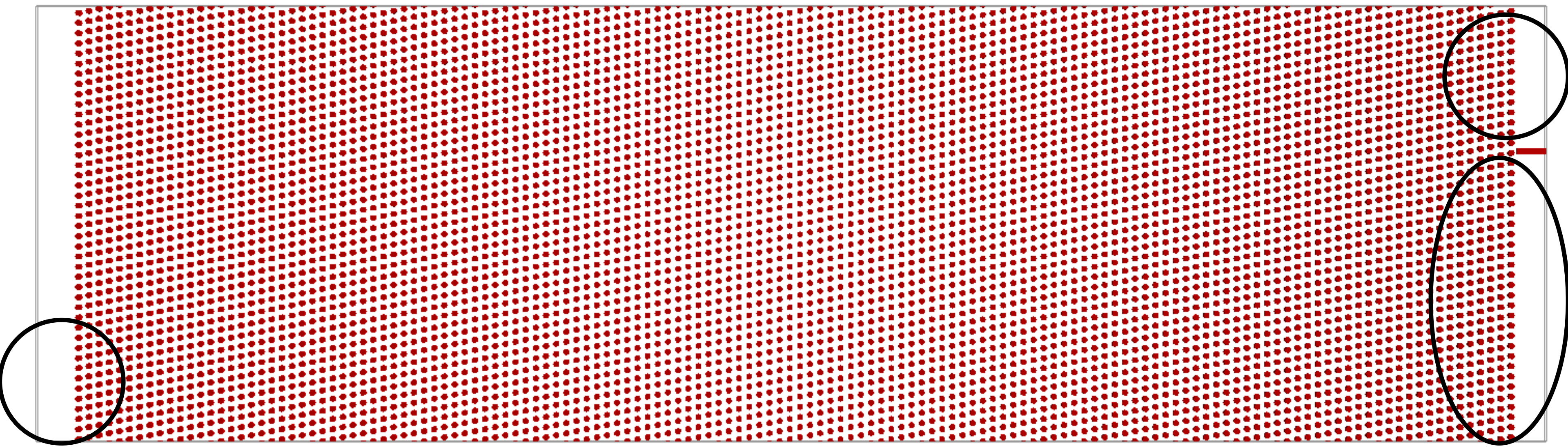
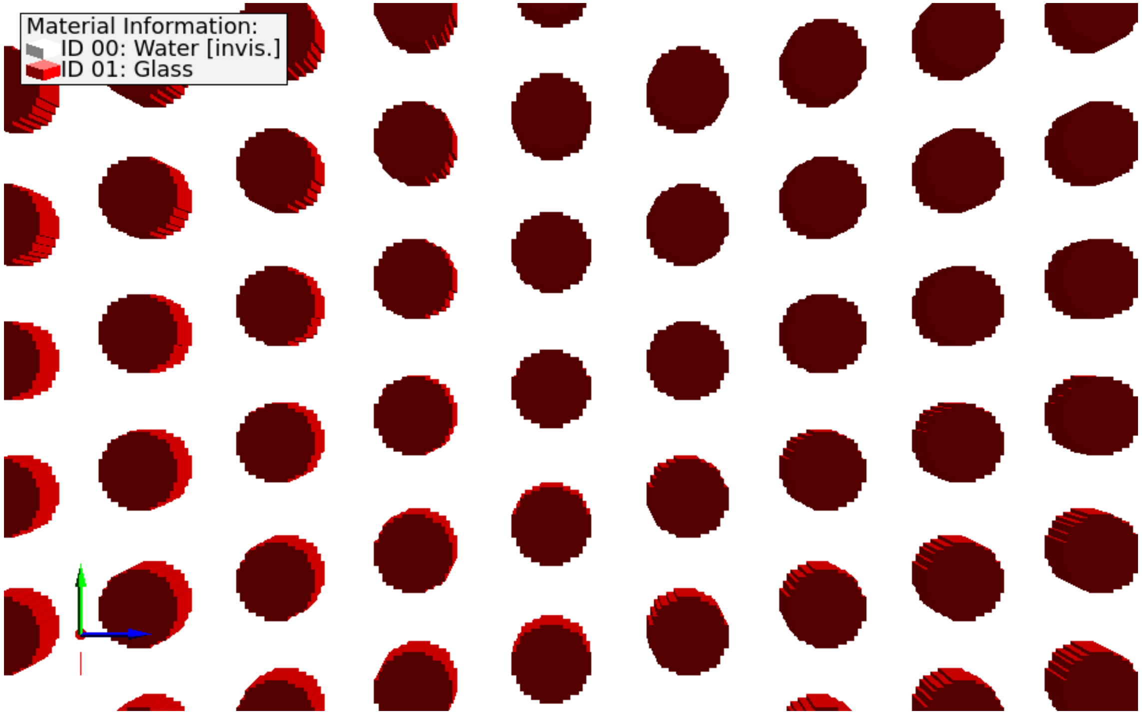
Results - DLD

- Virtual design of a DLD device
- Height $1.5\ mm$, width $5.2\ mm$ (including inlet and outlet), thickness $0.02\ mm$
- Particles enter in a channel of height $0.5\ mm$ at the left bottom
- Separation on the left by height



Results – DLD (cont.)

- Size of post $20\ \mu m$, size of gap $15\ \mu m$, deflection $11.31°$
- Critical particle diameter is $\sim 8\ \mu m$



Results DLD (cont.)

- The small deflection angle requires the width of the device

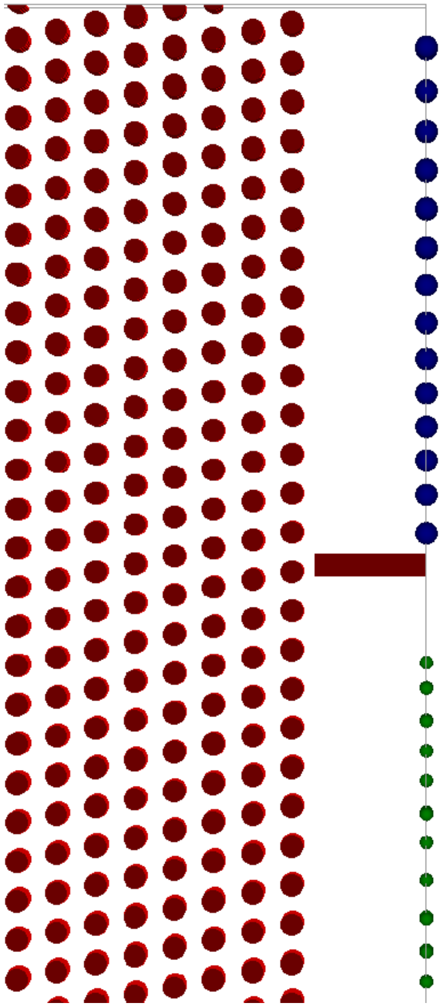
$$width = height/\tan(deflection\ angle)$$

- In our case a width of $5000\ \mu m$ (+inlet and outlet) is required
- For smaller height also inflow channel get smaller

  -> less throughput

Results – DLD (cont.)

- Pressure drop $595.74\ Pa$
- Separation efficiency (as designed) 100%
  (particles enhanced in picture)
- Large particles directed to the top of the domain, small particles stay at the lower part



Summary and conclusions

Summary:

- Investigation of the influence of different factors on the filtration efficiency and pressure drop
- Comparison to DLD

Conclusions:

- Porosity and surface area no suitable indicators for predicting the particle capturing efficiency
  - Pore size is a better indicator
  - Morphology of the structure is also more important
- Porosity and pore size influence pressure drop
- In comparison to DLD $100\ \%$ separation efficiency can not be achieved
  - But pressure drop much lower and higher throughput can be achieved

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Thank you for your attention!!!

Questions???

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