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A Multi-Physics Study of the Wave Propagation Problem in Open Cell Polyurethane Foams

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Huntsman Polyurethanes

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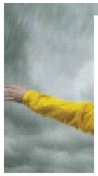
Huntsman Corporation

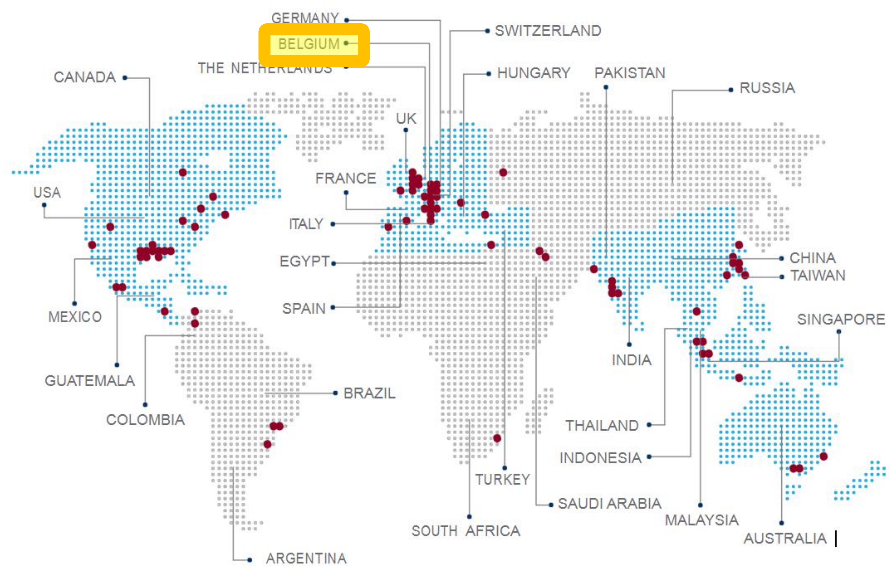
Introduction to our business

Polyurethanes	**Performance Products**	**Advanced Materials**	**Textile Effects**
MDI	Amines	Composites	Dyes
Polyols	Surfactants	Adhesives	Chemicals
PO/MTBE	Maleic Anhydride	Resins	Apparel
TPU	Upstream Intermediates		Home & Institutional
PU Systems			Technical Textiles



more than 75 manufacturing, R&D and operations facilities in over 30 countries;

approximately 10,000 associates.



2016

Revenues
$9.6
billion

Adjusted EBITDA
$11.2
billion

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Introduction to Research & Development

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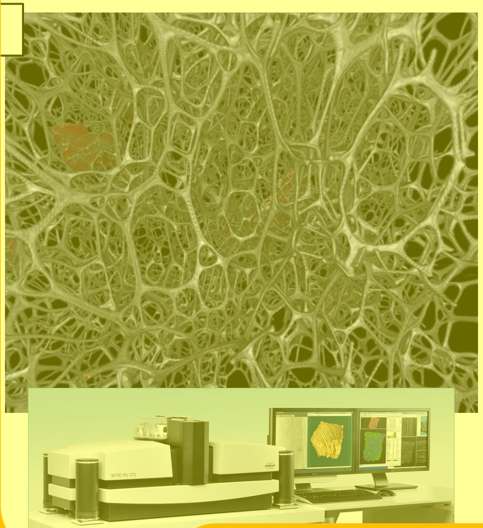
PU chemistry | **Foam cell morphology** | **Foam macro-properties** | **Market application**

Polyol

Isocyanat

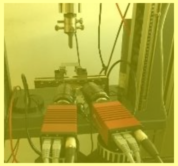
Polyurethane



Foam Characterisation

Acoustic laboratory

Dynamic mechanical analysis

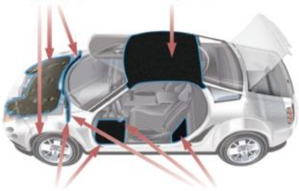


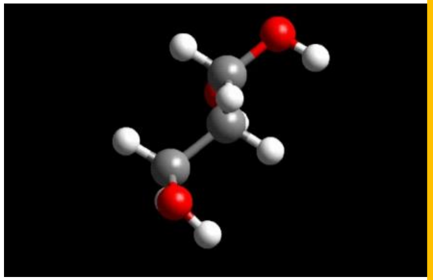
X-ray tomography

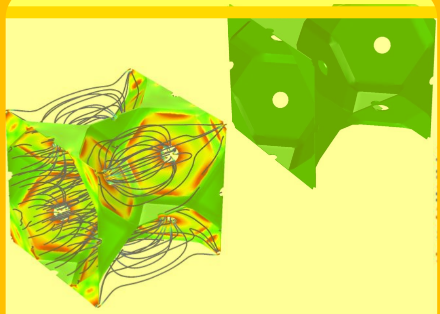
Digital Imaging Correlation

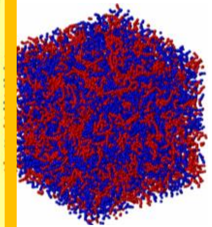
Alpha cabin

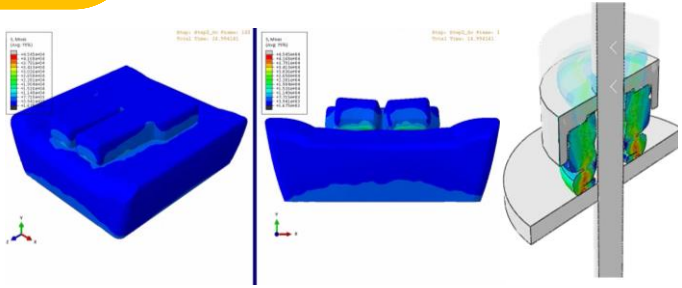
- ✓ Adhesives, Coatings and Elastomers
- ✓ Appliances
- ✓ Automotive
- ✓ Insulation
- ✓ Composite Wood Products
- ✓ Footwear
- ✓ Furniture & Bedding
- ✓ TPU











Molecular scale | Meso scale | Micro scale | Macro scale

A multi-scale modelling challenge

Huntsman Polyurethanes

Why is the study of wave propagation important in PU foams?

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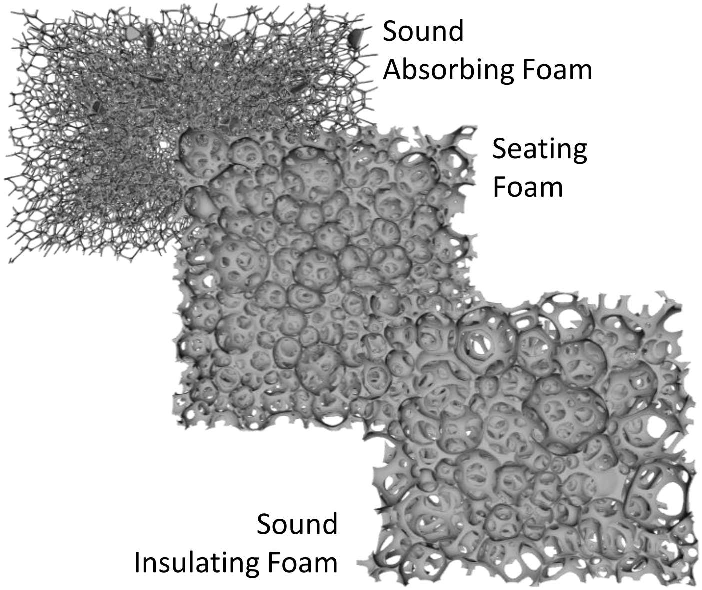
PU chemistry

Polyol
Polyether
Polyester

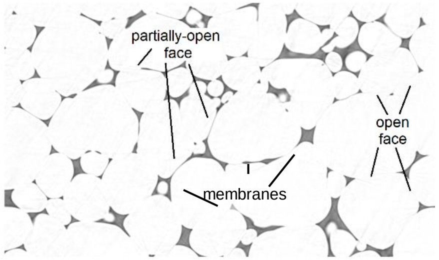
Isocyanate
Polymeric
MDI
Pure MDI
TDI

Polyurethane
Rigid foam
Flexible foam
Elastomeric foam
Adhesives
Thermoplastic urethanes (TPU)

Foam cell morphology



Micro-CT reconstruction of flexible foam



2D micro-CT image of flexible foam

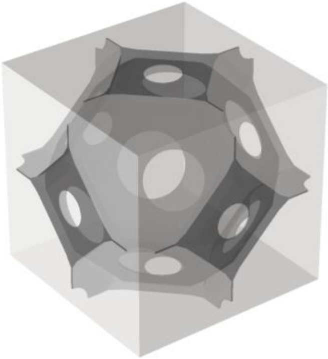
Foam properties depend on:
i. **Foam microstructure** and **permeability**;
ii. Polymer viscoelasticity;
iii. **Foam fluid-structure interaction**.

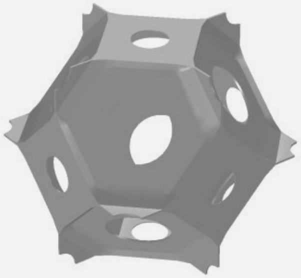
<u>Aim of the work</u>

To predict **foam permeability** (2D reference and 3D Kelvin models) and to study the **effect of cell face membranes** on wave propagation through PU foam, modelling the coupling between air- and structure-borne wave propagation.

Problem Formulation

Fluid-Structure interaction





Cellular microstructure domain

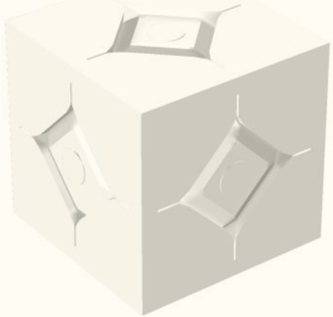
Linear-elastic material

$$\rho_s \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot \sigma = \mathbf{F}_s$$

Effect of structural vibrations on the fluid velocity

⟺

Fluid pressure on the solid domain



Air domain

No inertial term
Slow air flow through open cells

$$\rho_f \frac{\partial \mathbf{v}}{\partial \mathbf{t}} = \nabla \cdot \left[-p\mathbf{I} + \mu\left(\nabla \mathbf{v} + \nabla \mathbf{v}^{\mathrm{T}}\right)\right] + \mathbf{F}_{\mathrm{f}}$$

$$\rho_f \nabla \cdot \mathbf{v} = \mathbf{0}$$

Fluid-structure coupling equations

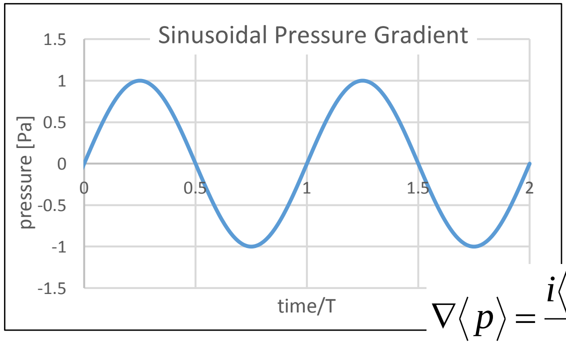
$$\mathbf{v} = \frac{\partial \mathbf{u}}{\partial \mathbf{t}}$$

$$\sigma \cdot \mathbf{n} = \left[-p\mathbf{I} + \mu\left(\nabla \mathbf{v} + \nabla \mathbf{v}^{\mathrm{T}}\right)\right] \cdot \mathbf{n}$$

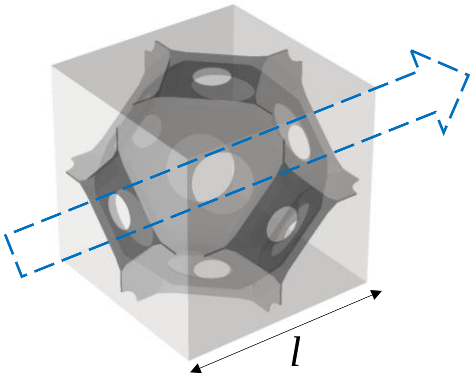
+ boundary conditions

Problem Formulation

Pressure gradient and average velocity in PU foams



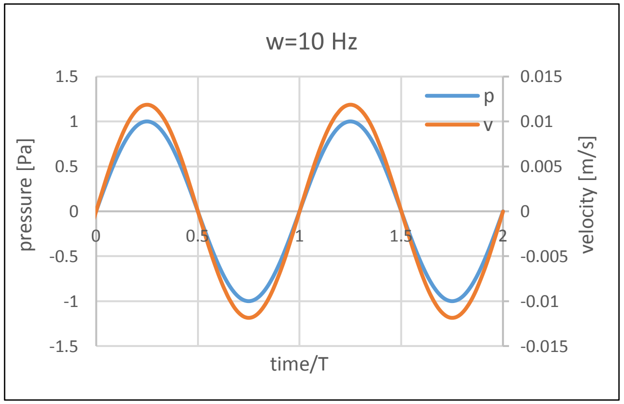
$$\nabla\langle p\rangle = \frac{i\langle P_0\rangle e^{iwt}}{l}$$

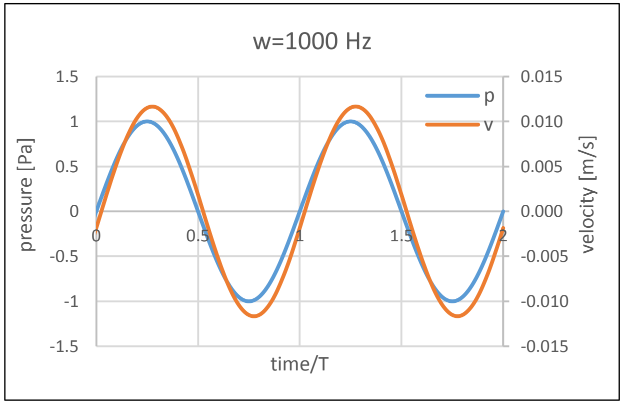


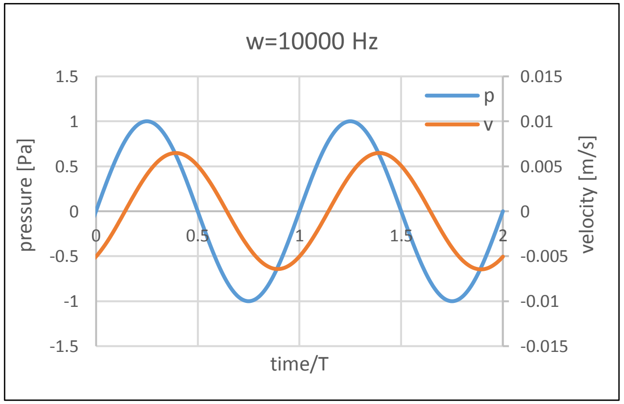
Within a few cycles the average velocity (flow) will oscillate at the same frequency, but will be shifted by a phase angle φ with respect to the pressure gradient.

$$\nabla\langle v\rangle = -i\langle v_0\rangle e^{i(wt+\varphi)}$$

Increasing w, the frequency of pressure gradient.





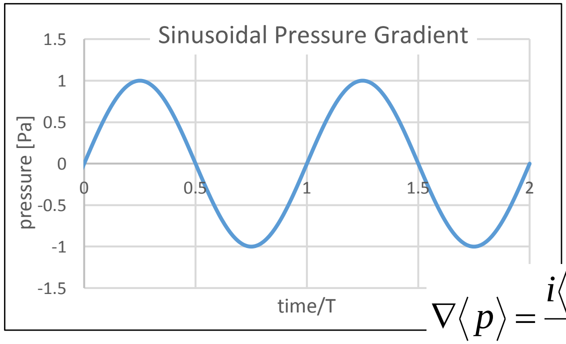


$\langle v_0\rangle$, amplitude of velocity, decreases
φ, the shift angle, increases

Brennan et al., *Acta Acust united Ac,* (2010)

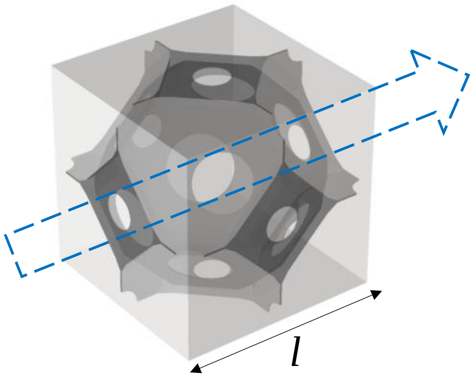
Problem Formulation

Mathematical model of dynamic viscous permeability in PU foams



$$\nabla\langle p\rangle = \frac{i\langle P_0\rangle e^{iwt}}{l}$$

$$\nabla\langle v\rangle = -i\langle v_0\rangle e^{i(wt+\varphi)}$$



Darcy's law for porous materials

⇩

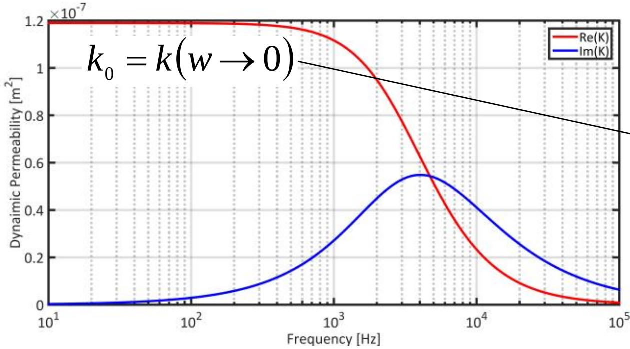
defines the relationship between the **average pressure gradient** and the **average velocity** by means of the **permeability**

$$k(w) = -\mu\frac{\langle v\rangle}{\nabla\langle p\rangle} = \mu\frac{\langle v_0\rangle}{i\langle P_0\rangle / l}e^{i\varphi}$$

$$k(w) = k' + k'' = |k|\cos(\varphi) + |k|\sin(\varphi)$$

real part + imaginary part

Real and imaginary parts of dynamic permeability



The frequency response of the real and imaginary parts of the permeability will depend on the **foam cell morphology**.

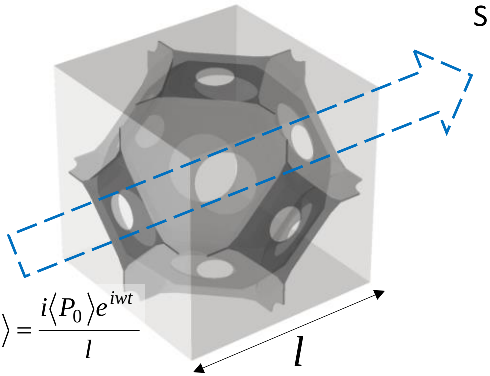
The **static permeability** is related to **flow resistivity**

$$k_0 = \frac{\mu}{\sigma_0}$$

measure with an air flow resistivity experiment

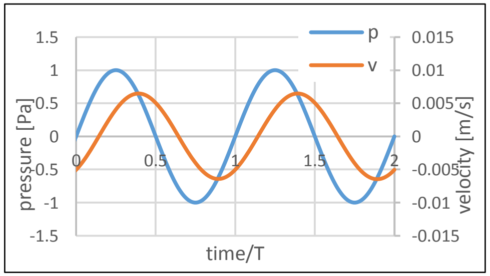
Problem Formulation

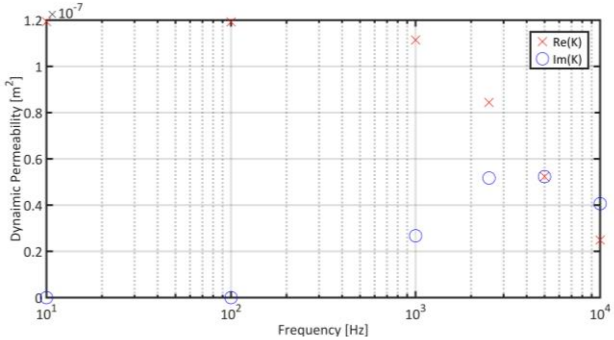
How are the real and imaginary parts of dynamical permeability obtained?

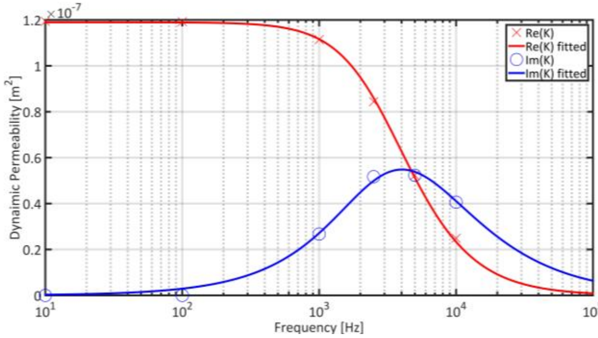


$$\nabla\langle p\rangle = \frac{i\langle P_0\rangle e^{iwt}}{l}$$

Simulation performed only at few frequencies







Wilson's model of sound propagation of porous material has been used to fit results and obtain dynamic permeability

$$k(w) = \frac{\mu}{\alpha_\infty \rho_f i w}\left(1 - \sqrt{1 - \frac{i w k_0 2 \rho_f \alpha_\infty}{\mu}}\right)$$

Brennan et al., *Acta Acust united Ac,* (2010)

Numerical example:

2D reference model: **rigid** cellular microstructure

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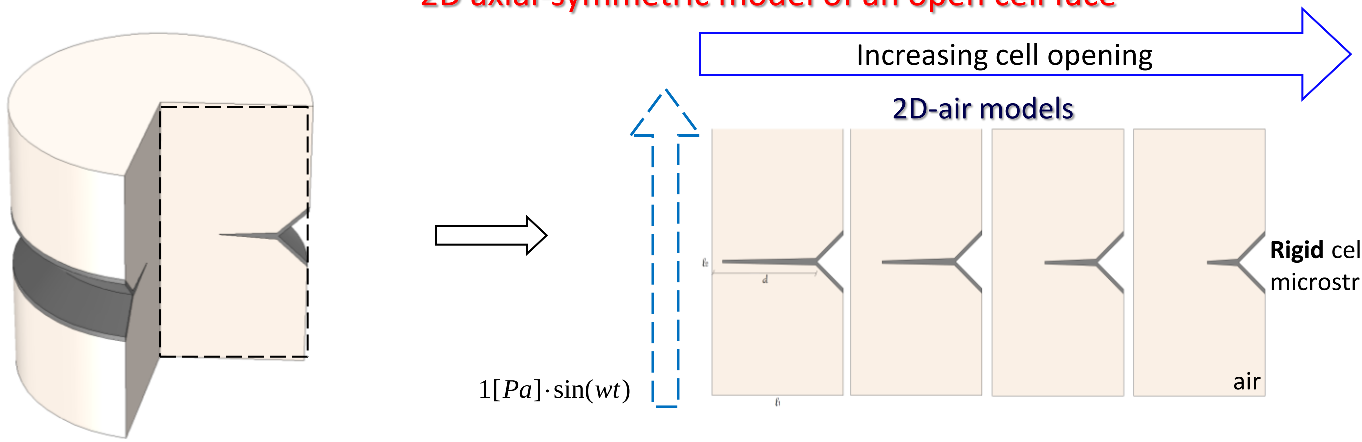
2D axial-symmetric model of an open cell face



Increasing cell opening

2D-air models

Rigid cellular microstructure

air

$1[Pa] \cdot \sin(wt)$

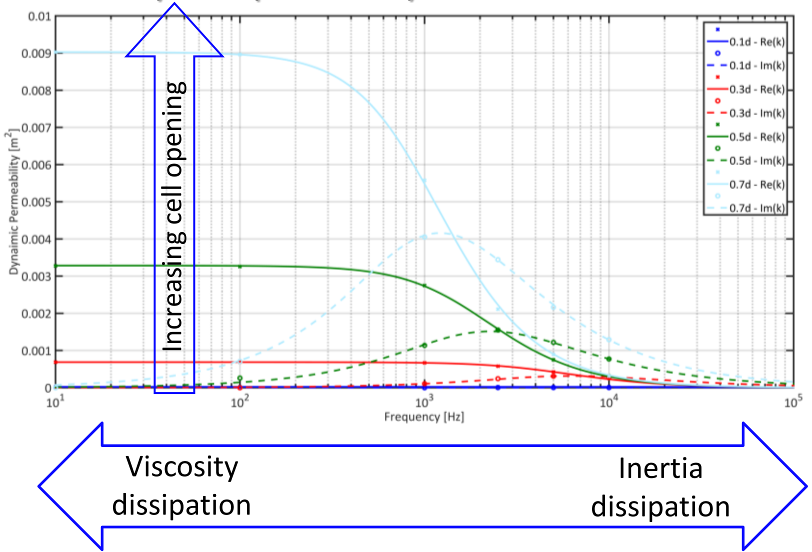
$d = 1.22 \cdot 10^{-4}$ m

$\rho_f = 1.29 \, \text{kg}/\text{m}^3$

$\mu = 18 \cdot 10^{-6}$ Pa·s

Air-borne wave propagation

Dynamic permeability – simulation results

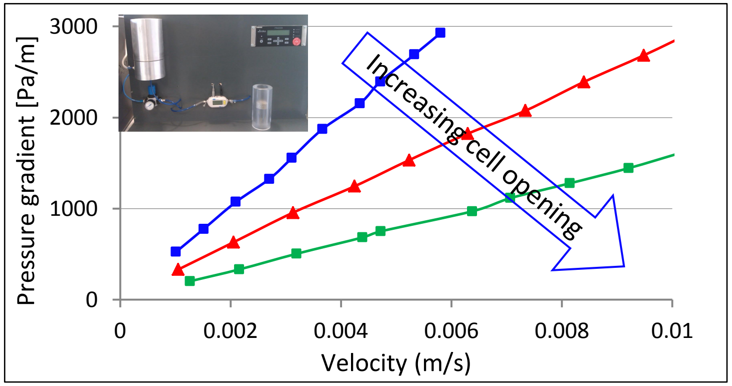


Increasing cell opening

Viscosity dissipation

Inertia dissipation

Airflow resistivity – experimental results of PU flex foams



Increasing cell opening

$$k_0 = \frac{\mu}{\sigma_0}$$

Simulation results are qualitatively confirmed by the experimental results.

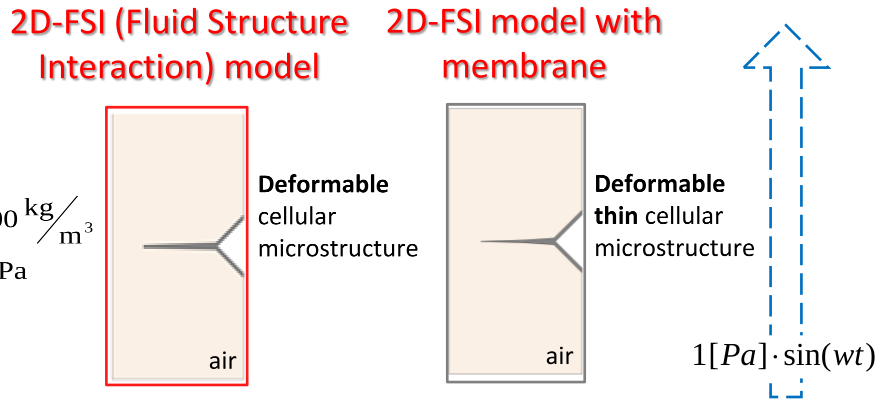
Numerical example:

2D reference model: *membrane* effect

$\rho_s = 1100 \, {}^{\text{kg}}/_{\text{m}^3}$

$E = 10^8 \text{ Pa}$

$\nu = 0.45$



cell opening = 0.3*d*

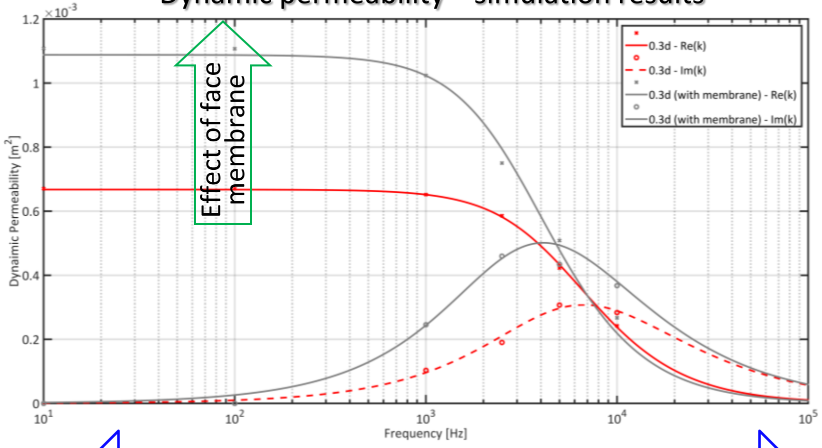
The bending of the **cell face membrane** allows more fluid to flow through the cell.

Such effect is similar to an increasing of cell opening ratio.

The effect is negligible at high frequency.

Fluid-structure interaction – Membrane effect

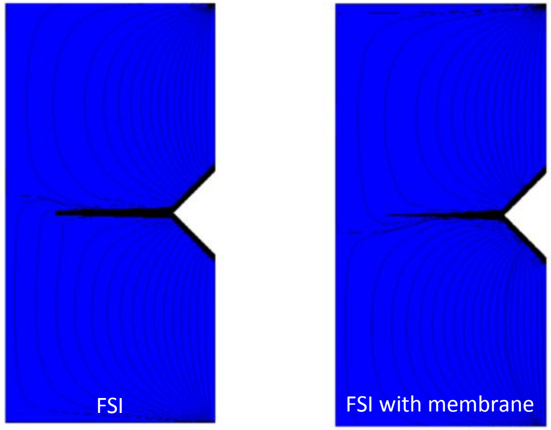
Dynamic permeability – simulation results

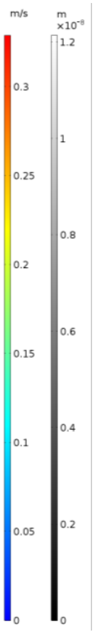


Viscosity dissipation

Inertia dissipation

w=10 Hz





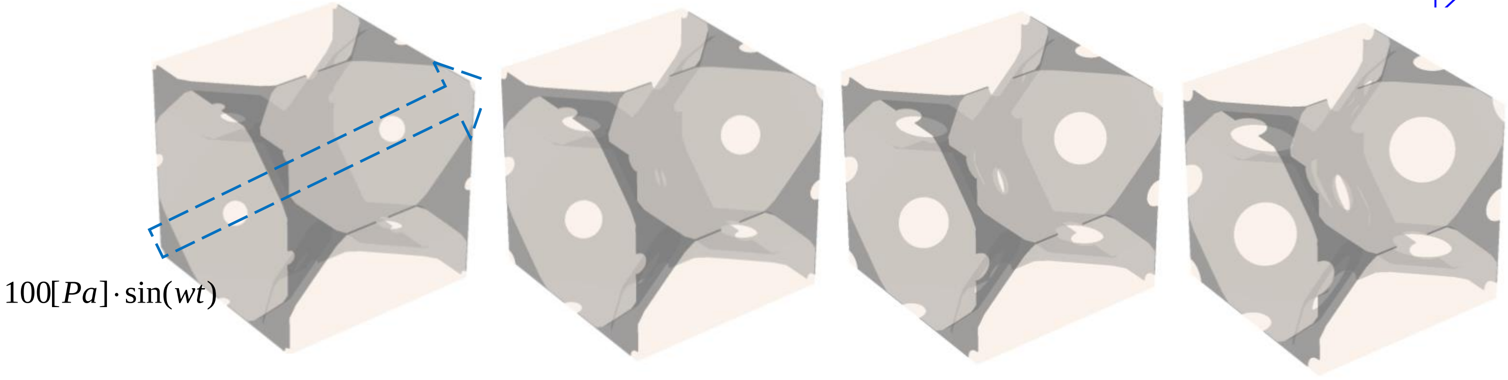
Maximum cellular microstructure deflection:

$2.8 \cdot 10^{-6}$ mm $\quad$ $1.2 \cdot 10^{-5}$ mm

Numerical example:

3D kelvin cell model

Increasing cell opening



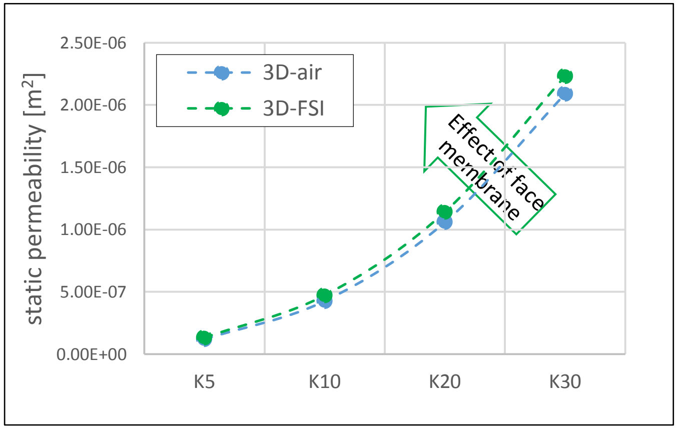
$$\rho_s = 1100\ {}^{\mathrm{kg}}\!/_{\mathrm{m}^3}$$

$$E = 10^8\ \mathrm{Pa}$$

$$\nu = 0.45$$

Fluid-structure interaction – Membrane effect

Static permeability



Increasing cell opening

The 3D model agrees what found in 2D reference model.

The fluid pressure triggers the vibration of the thin solid membranes. This increases the fluid flow through the cell.

Numerical example:

3D kelvin cell model: K5 – *membrane effect*

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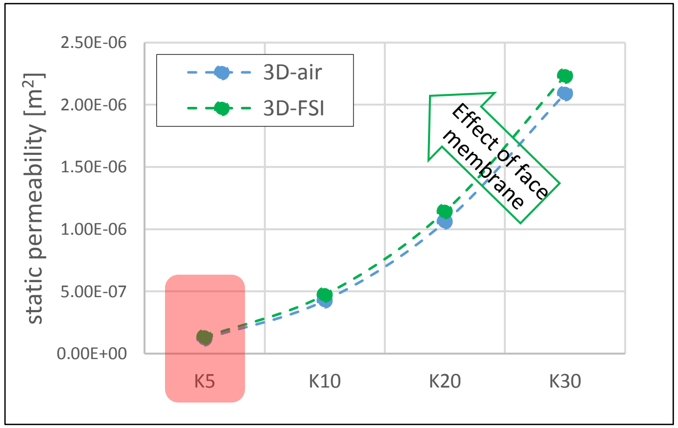
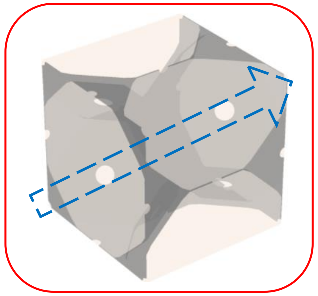
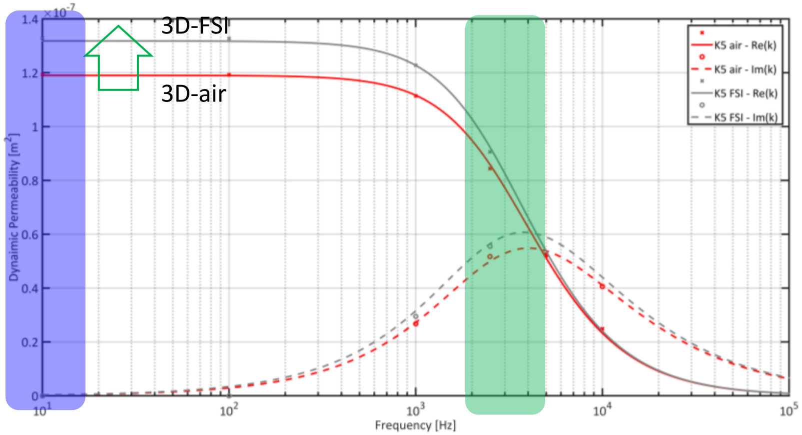
Static permeability

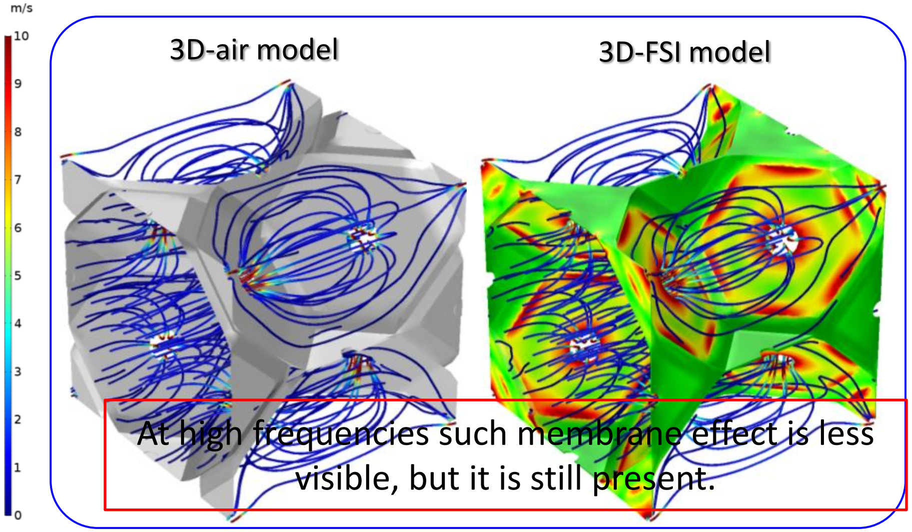


Increasing cell opening

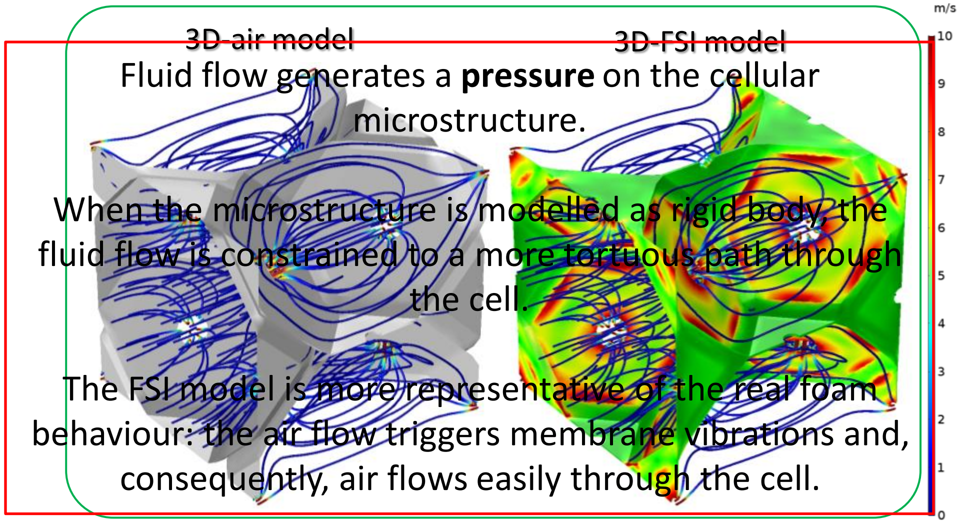


Dynamic permeability





At high frequencies such membrane effect is less visible, but it is still present.



Fluid flow generates a **pressure** on the cellular microstructure.

When the microstructure is modelled as rigid body, the fluid flow is constrained to a more tortuous path through the cell.

The FSI model is more representative of the real foam behaviour: the air flow triggers membrane vibrations and, consequently, air flows easily through the cell.

Numerical example:

3D kelvin cell model: cell opening and frequency effects

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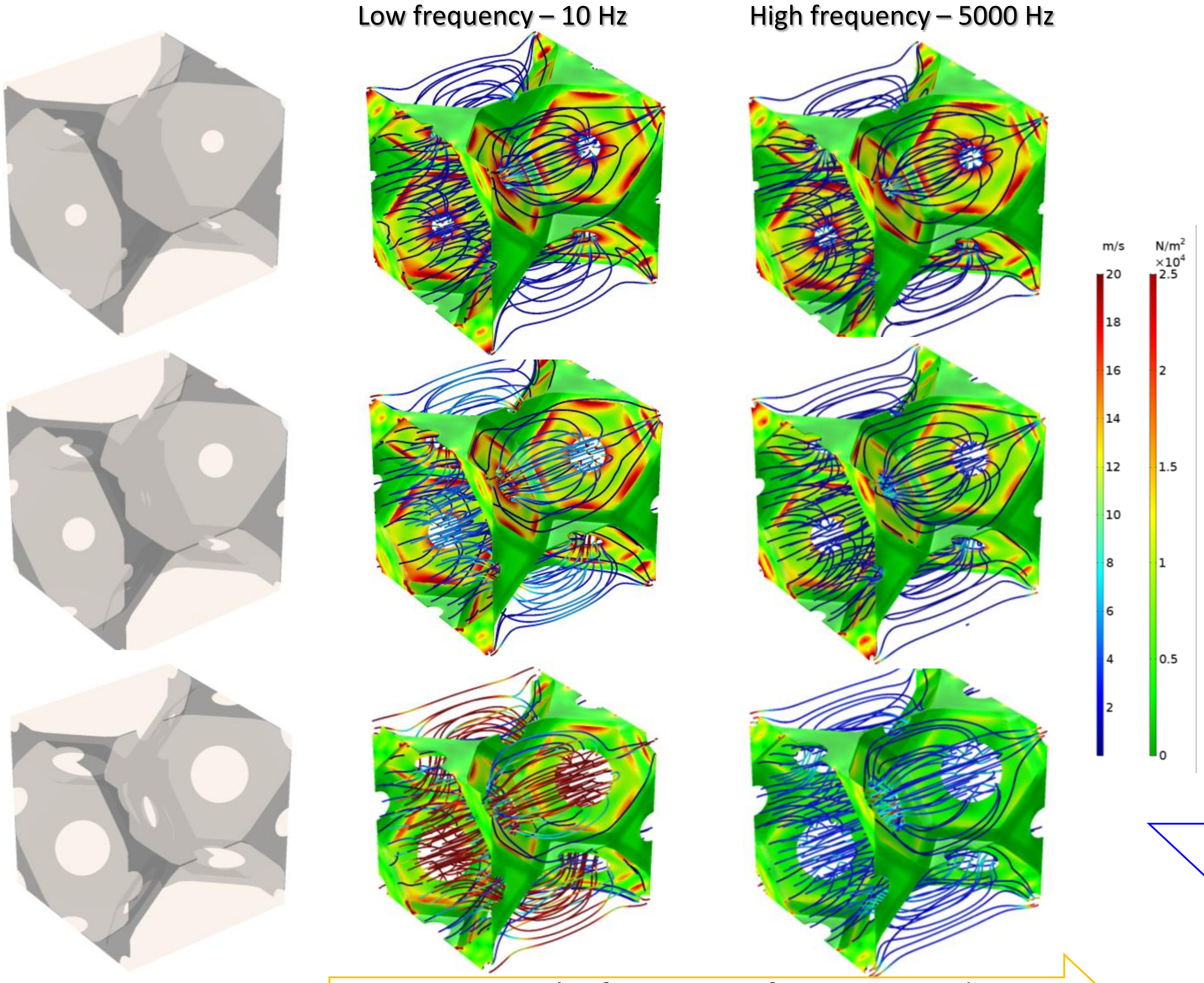
Increasing cell opening



Low frequency – 10 Hz

High frequency – 5000 Hz

<u>Increasing cell opening</u>

Air flow increases;

Stress concentrations are located more close to the structures than on the cell faces.

<u>Increasing the frequency of pressure gradient</u>

Stress concentrations and velocity flow decrease.

Numerical example:

3D kelvin cell model: vibrations amplitude

Smaller the cell opening is, bigger vibration amplitude of the thin membrane;

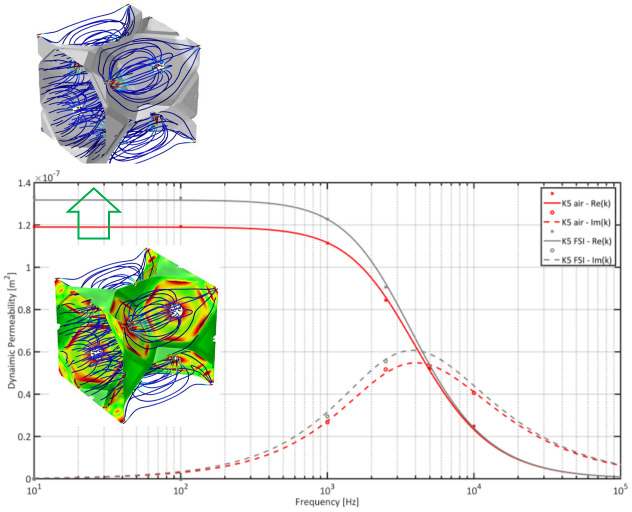
The maximum membrane deflections are located along the hole borders.

Low frequency – 10 Hz

Conclusions

COMSOL Multiphysics has been used to study wave propagation problem in PU foams; **FSI** is necessary to study the effect of cell face membranes;

The main factors influencing the **foam permeability** are **size** and **cell hole area**; increasing the cell opening ratio, the static permeability increases.



Vibrations of the **thin membranes** have a similar effect to larger cell opening; air flows less tortuously through the foam cell, and the static permeability increases.

Membrane effect is negligible at high frequencies, where the **viscous dissipation** decreases and the drag that the solid structure exerts on the fluid is dominated by inertia effects.

Thank you for your attention.

Acknowledgements

Rajesh Gajendran for the airflow data

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Permeability Tensor

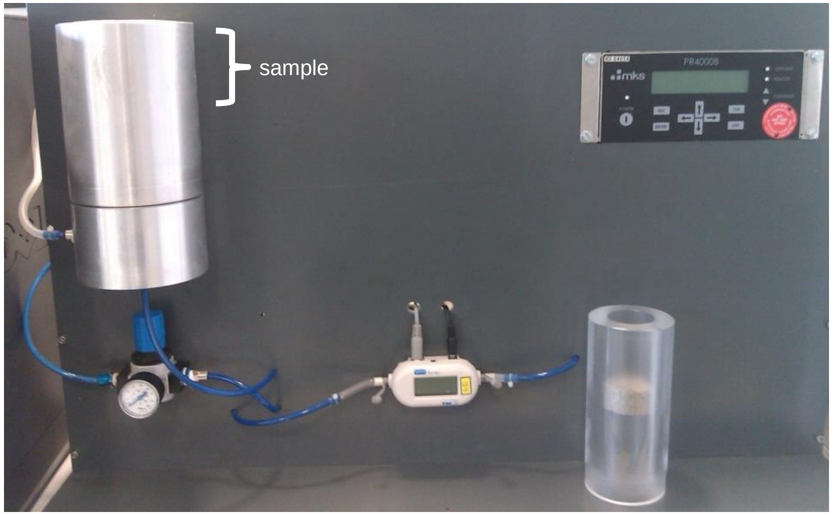
- Permeability characterises the ease with which a fluid can flow through a porous medium, e.g., an open cell foam
  - It is inversely proportional to the air flow resistance for isotropic foam, $K = \mu / \sigma$

- The permeability of a foam is a function of the foam cell morphology
  - Foam cell network, foam density, foam cell size distribution and degree of cell opening

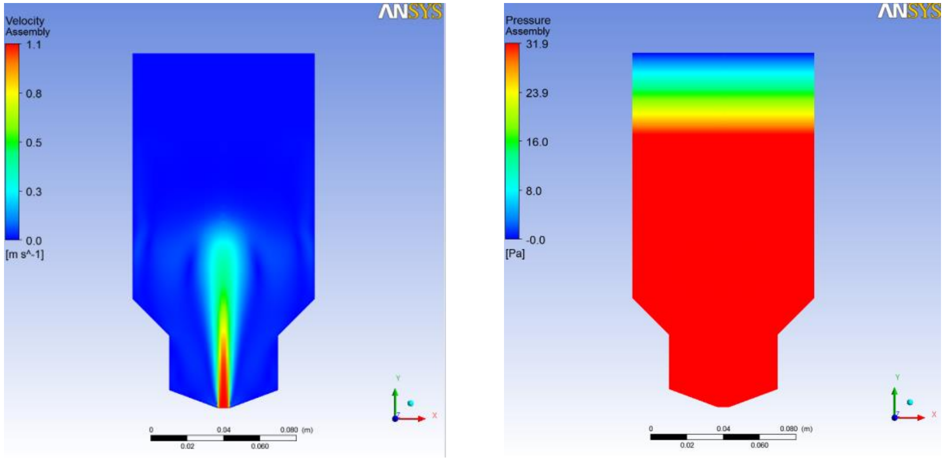
- For <u>anisotropic</u> foam permeability is a tensor providing the geometric relationship between the fluid flow and the pressure gradient

$$\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = -\underbrace{\frac{1}{\mu}\begin{pmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{pmatrix}}_{\text{Permeability tensor}}\begin{pmatrix} \partial P/\partial x \\ \partial P/\partial y \\ \partial P/\partial z \end{pmatrix}$$

Air Flow Measurements of Foams



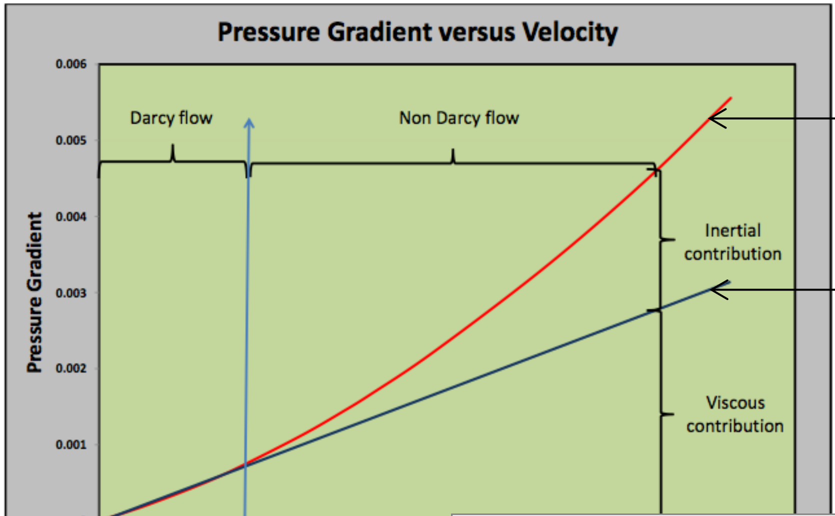
Air flow meter



CFD simulations results: flow and pressure

- Static air flow resistance is measured as a ratio of the pressure gradient and the average speed, $\sigma = \nabla p \,/v$
  - For acoustic foams the range of values for the static air flow resistivity is approximately 10^3 – 10^6 N s m^{-2}
  - It is also a measure of the degree of cell opening in a foam

Darcy’s and Forchheimar’s equations

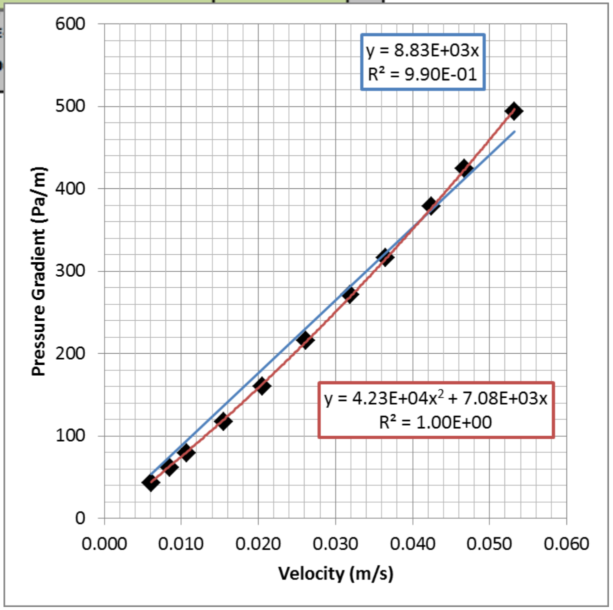


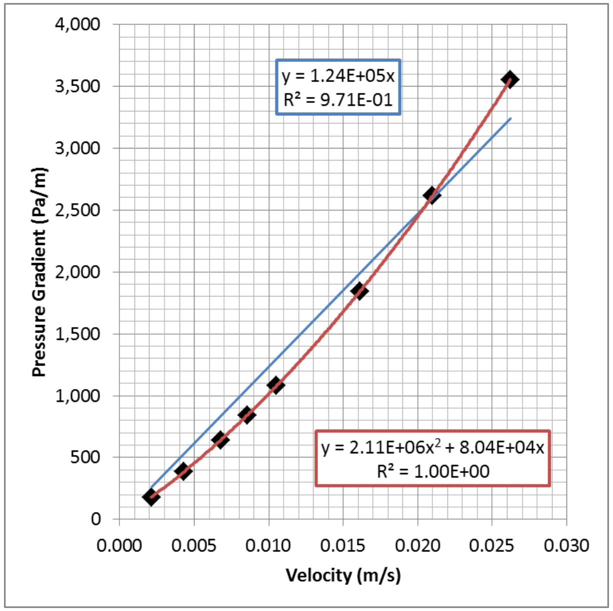
$$\nabla p = \sigma v + \tau_{v}^{2}$$

Forchheimar’s relation

$$\nabla p = \sigma v$$

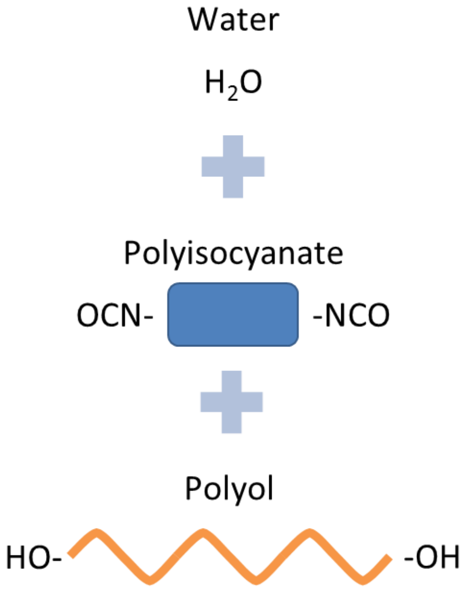
Darcy’s law





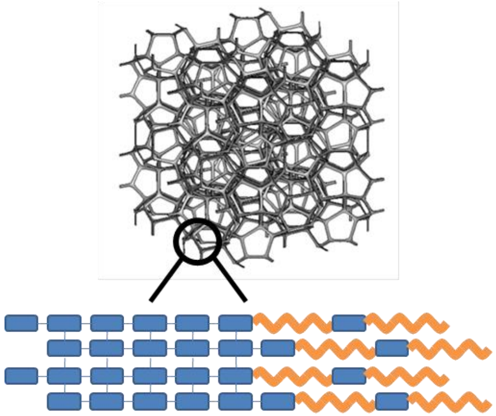
Acoustiflex foam samples

Mechanical Representation of Flexible Foam

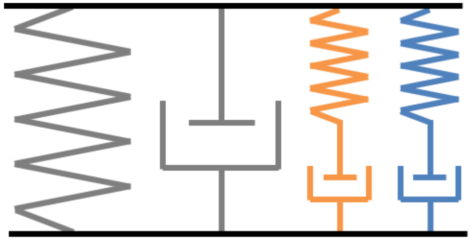


Polyurethane chemistry

Foam cellular microstructure

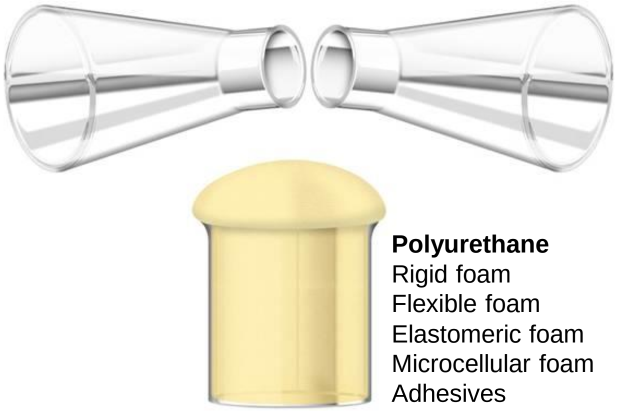


Hard and soft phase separated nanostructure



Mechanical equivalent model of Polyurethane foam

Polyol
Polyether
Polyester
Recycle PE
Formulations



Polyurethane
Rigid foam
Flexible foam
Elastomeric foam
Microcellular foam
Adhesives
Thermoplastic urethanes (TPU)

Isocyanate
Polymeric MDI
Pure MDI
TDI
MDI variants
Pre-polymers
MDI mixed isomers

Microstructural analysis of flexible polyurethane foam: Our experimental setup

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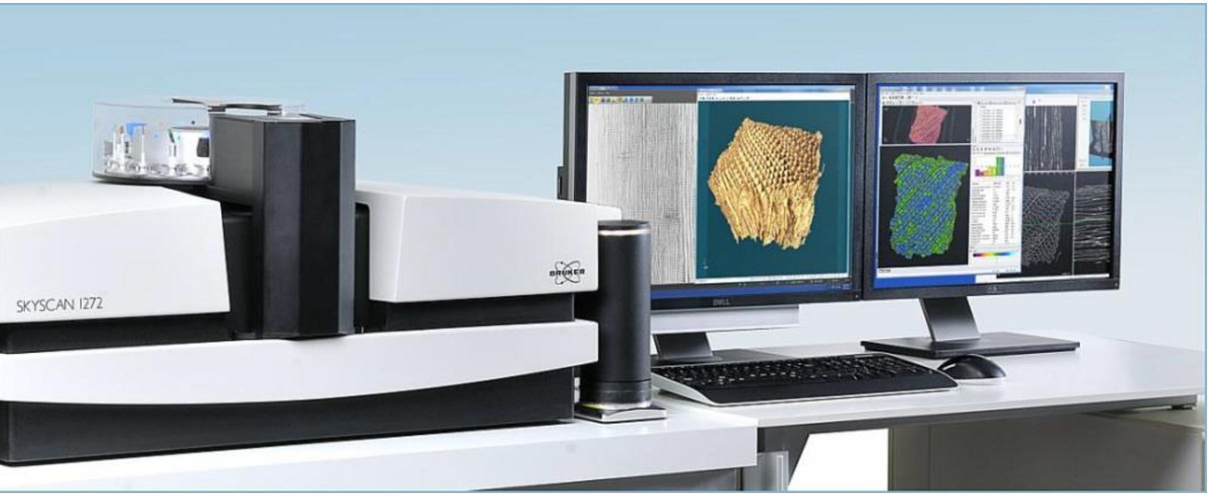
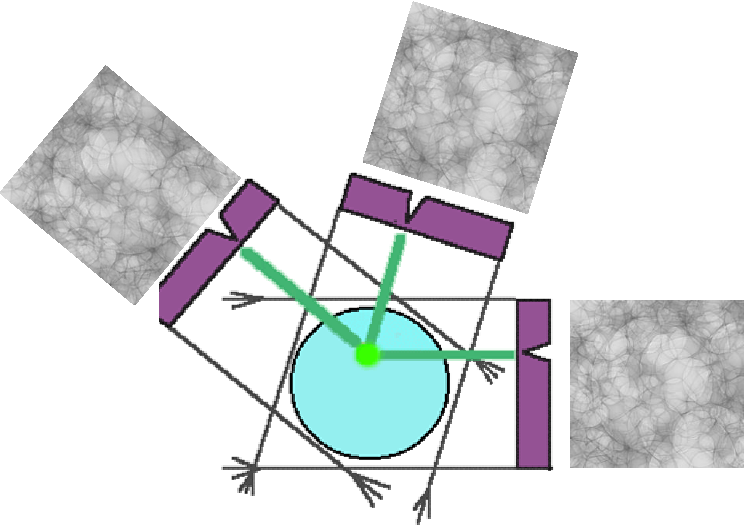
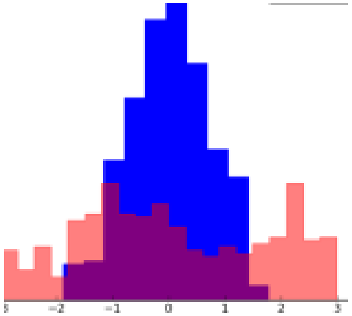
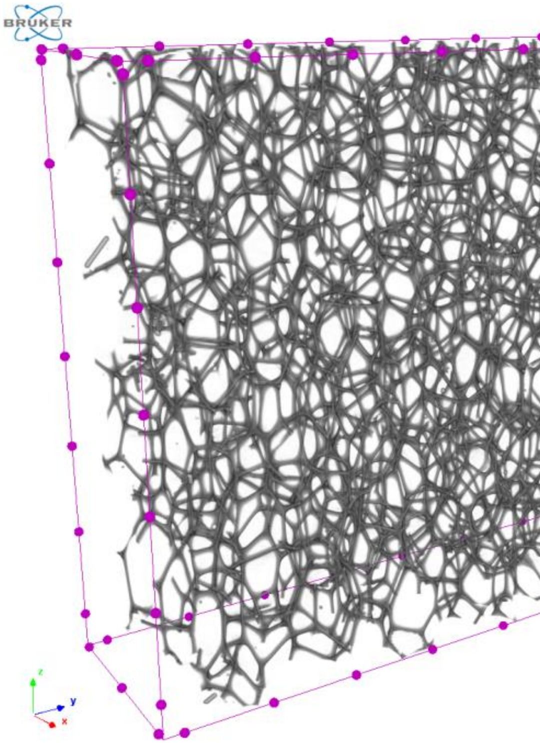


yscan 1272







Sample preparation → Scanning → 3D reconstruction →