VIRTUAL PROPERTY COMPUTATION AND DESIGN OF CERAMIC MATERIALS

ECerS
Torino, June 17th, 2019

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Math2Market GmbH, Kaiserslautern, Germany

Why am I here?

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- I am a Mathematician and CEO of a company (Math2Market), not a ceramics guy
- Math2Market makes software GeoDict, the digital material laboratory
  - Which creates geometric microstructure models
  - Can analyze the models for geometric properties
  - Can compute processes and material properties on these models
- This software has been used successfully for many different materials, and recently (by Willi Pabst and co-workers) also for ceramic materials
  - I think there is more potential to collaborate on ceramics, but am not an expert
  - And hence would like to introduce our capabilities to this audience

Our purpose as a company rather than an academic institution

GeoDict

- In everything that follows,
- Our intention is to make the technologies available to the audience
  - to speed up your modelling of processes and materials
  - to help you design new materials and processes
  - to understand the outcomes of real experiments
- In the best sense of reproducible research
  - by keeping software versions and input data with the results
  - by including the post-processing options used
- While making a living for ourselves
- If you find you'd like to know more after this presentation, talk to me after my presentation or visit our web site at www.geodict.com.

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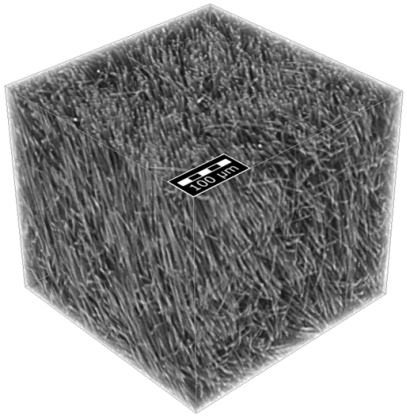
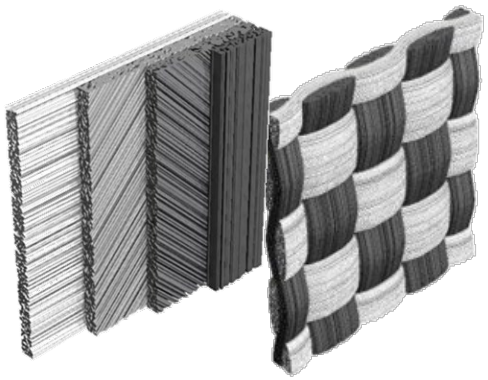
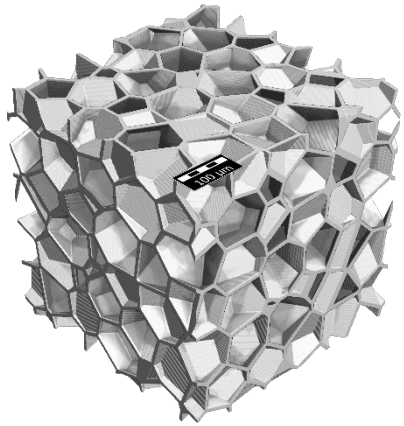
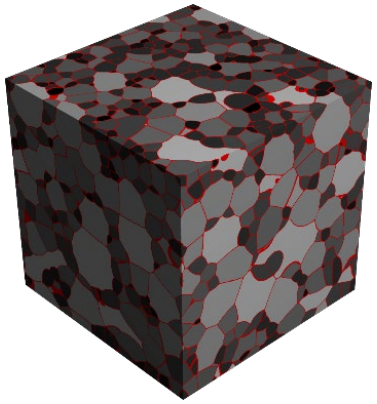
Modelling of Structural Materials

GeoDict









Import of image data	Generation of Composites	Generation of Foams	Crystalline materials
▪ µCT-scans, FIB-SEMs ▪ Slice alignment ▪ Curtain filter (FIB-SEM) ▪ Artifact Removal (µCT) ▪ OTSU-thresholding ▪ Median and mean filter ▪ Non-local means filter ▪ Gauss filter ▪ User defined filters	▪ Plain weaves ▪ Twill weaves ▪ Satin weaves ▪ Customized weaves ▪ Needle mats ▪ Short fibers ▪ Long fibers ▪ Non crimped fabrics	▪ Random foams ▪ Kelvin foams ▪ Closed cell foams ▪ Open cell foams ▪ Cell size distributions ▪ Foam beads ▪ Complex foam structures	▪ Metals and ceramics ▪ Generation of grains ▪ Different orientation of each grain ▪ Fiber reinforced ceramics ▪ Fiber reinforced metals ▪ Hybrid materials

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Digital Experiments on CT-Scans and Microstructures

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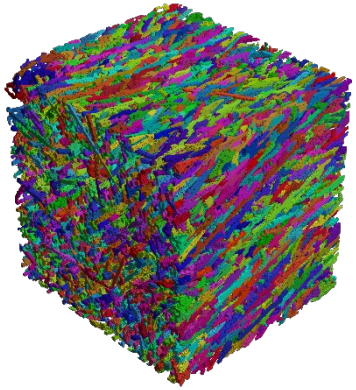

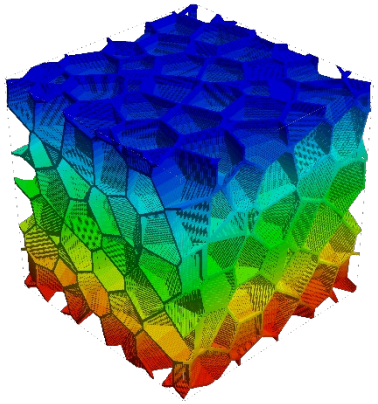

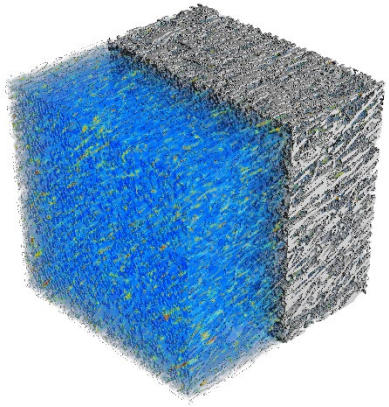

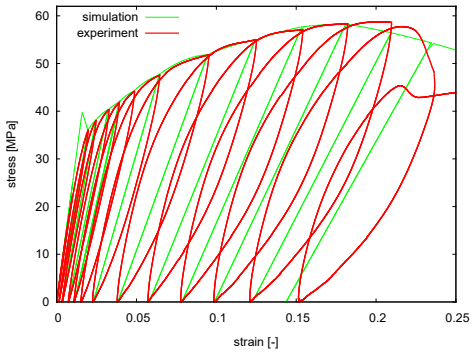

Geometrical Parameters	Flow & Conduction Parameters	Mechanical Parameters	Large Deformation, Damage & Failure
▪ Volume fractions ▪ Fibers, grains, pores ▪ Object diameters ▪ Object identification ▪ Object orientation ▪ Object size distributions	▪ Absolute permeability ▪ Thermal conductivity ▪ Electrical conductivity ▪ Tortuosity ▪ Diffusivity	▪ Elastic moduli ▪ Stiffness tensor ▪ Full anisotropy ▪ Thermal expansion ▪ Stress-strain curves	▪ Hyperelastic materials ▪ Plastic deformations ▪ Viscous effects ▪ Damage and failure ▪ Structure change ▪ Fatigue ▪ Buckling of cell walls

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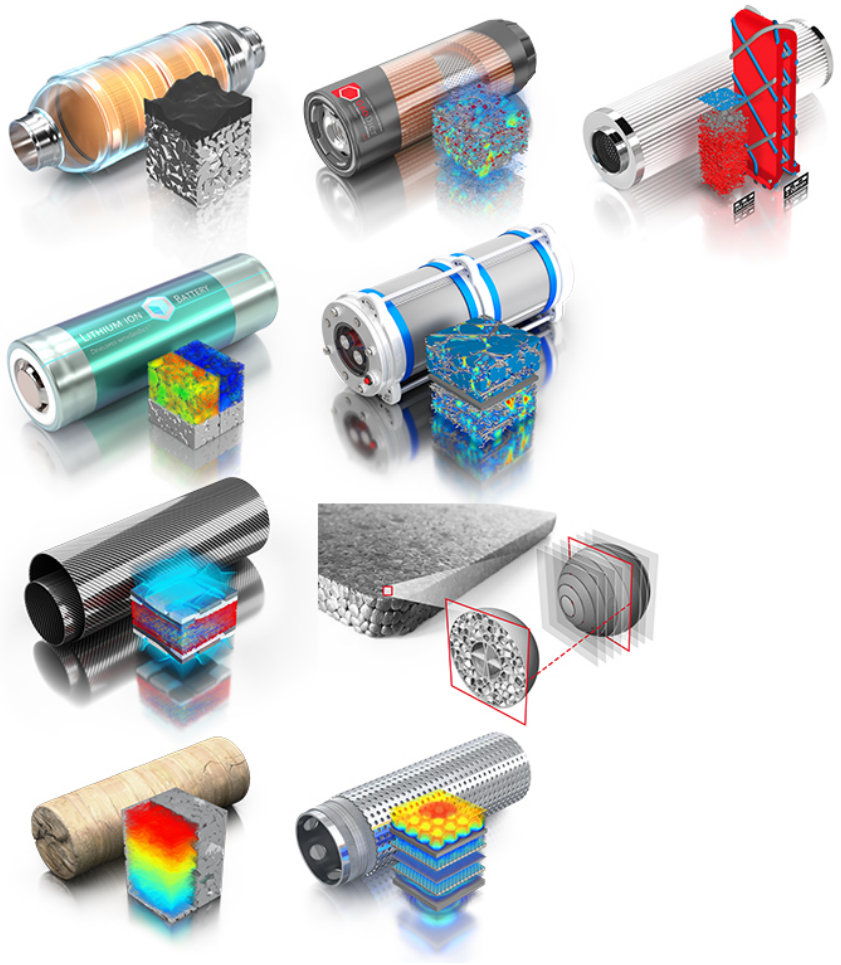
GeoDict® Solutions for ...

GeoDict

Filtration	For a clean environment
Electrochemistry	For electromobility
Structural materials	For lightweight applications
Digital Rock Physics	For efficient energy production



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Selected Clients

GeoDict

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What will you see?

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- Steps to develop a patent for a new Diesel Particulate Filter ceramic.
- Steps to develop a new washcoat for Three Way catalysts.
- Steps to validate and derive new cross-property relationships (and publish them).
- Ideas, what has been simulated on other materials and could be done on ceramics, too.

Introduction to Diesel Particulate Filters (DPF)

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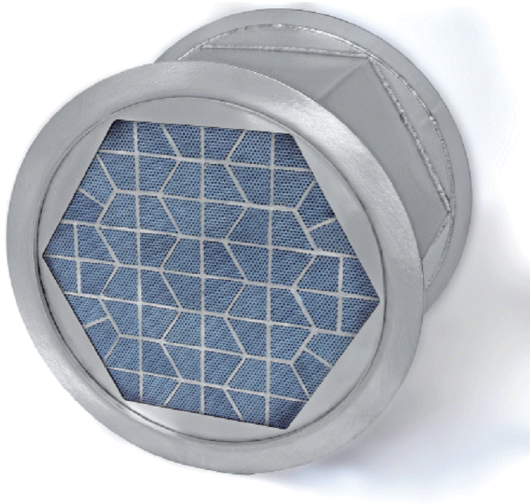
Goal:

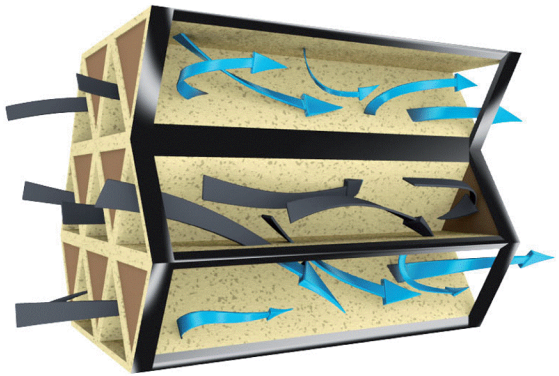
Design & improve Diesel/Gasoline Particulate Filters (DPF/GPF) through fast simulations.

- lower pressure drop
- higher filter efficiency
- improved regeneration



Key factor governing performance of the DPF:

Ceramic filter media



Two sources of pressure loss in DPF

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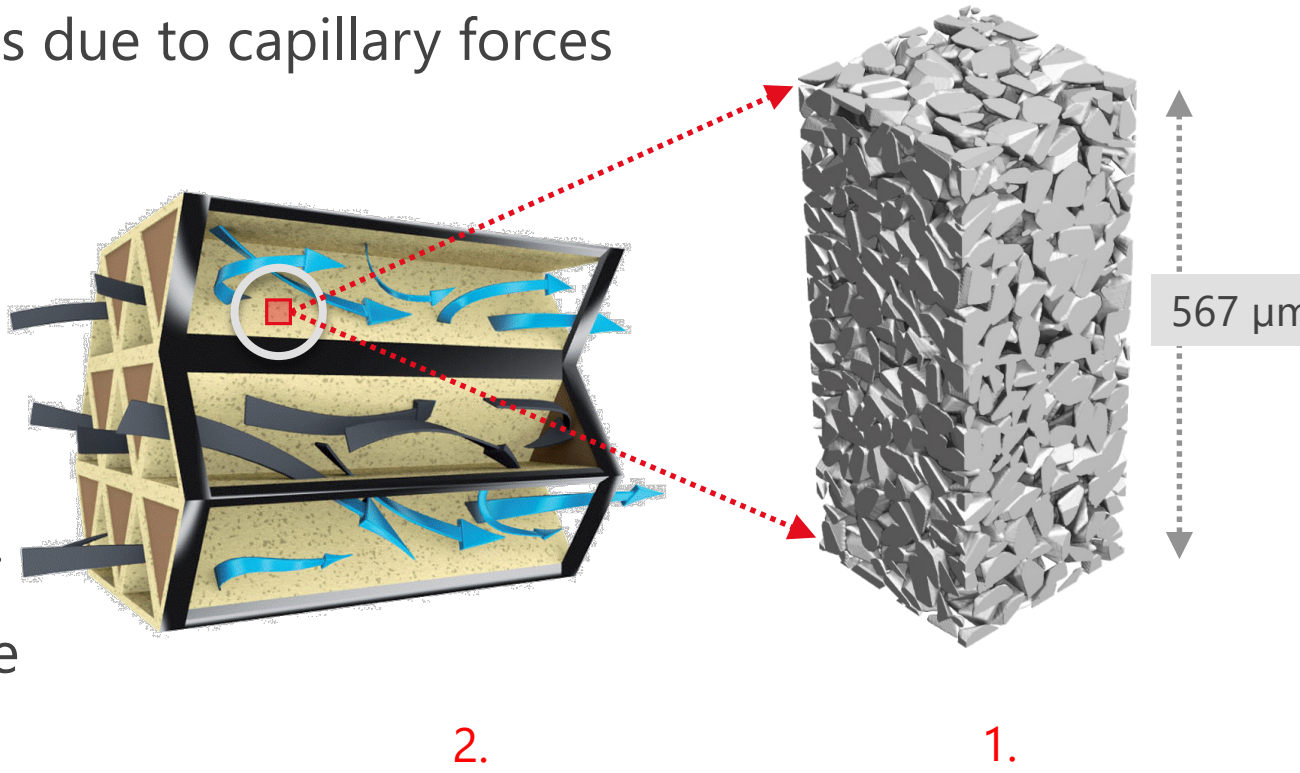
1. Across the ceramic micro structure
2. Along the channels due to capillary forces

- We simulate them separately.
- In both cases, we simulate the loading of an initially clean filter.
- After modeling the ceramic and
- After modeling the honeycomb.



PROCEDURE

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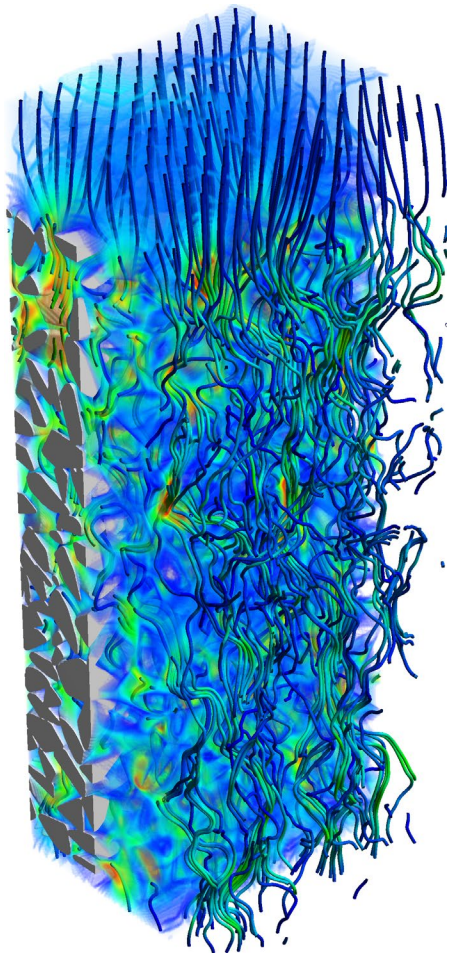
1. Simulate pressure loss across the wall
2. Simulate pressure loss along the channels



Micro-structure

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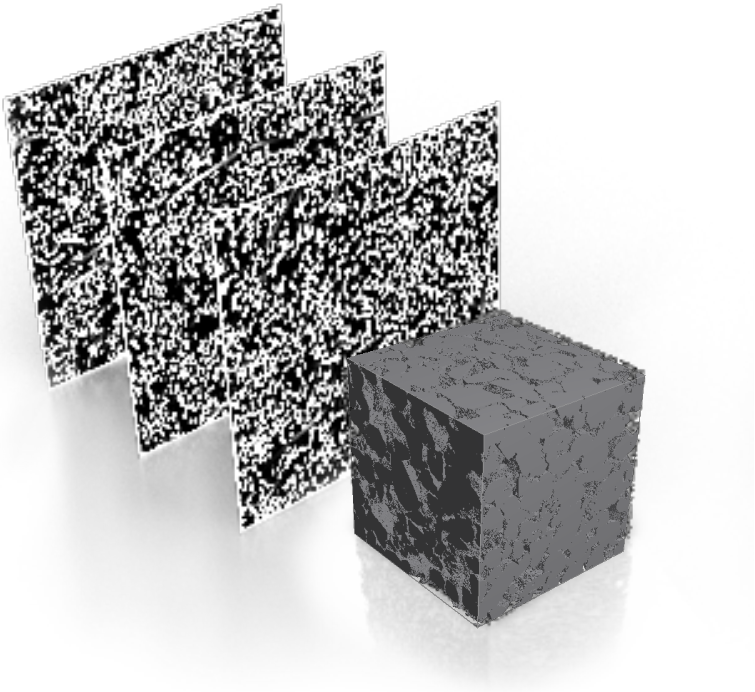

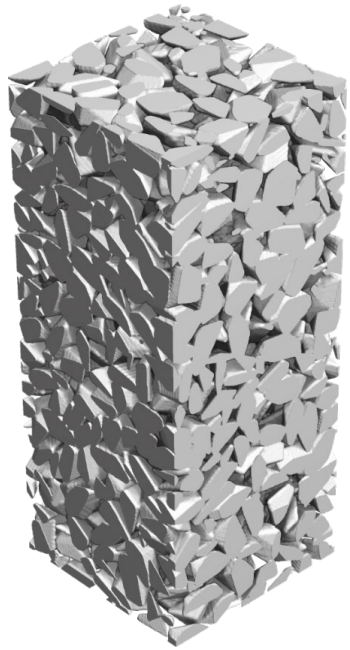

+ Allows simulations on real filter structures
− Modification of the filter structure is not possible only through µ-CT images

Modelling with **GeoDict**
structure generator modules,
e.g. GrainGeo

Micro-structure models with GrainGeo module

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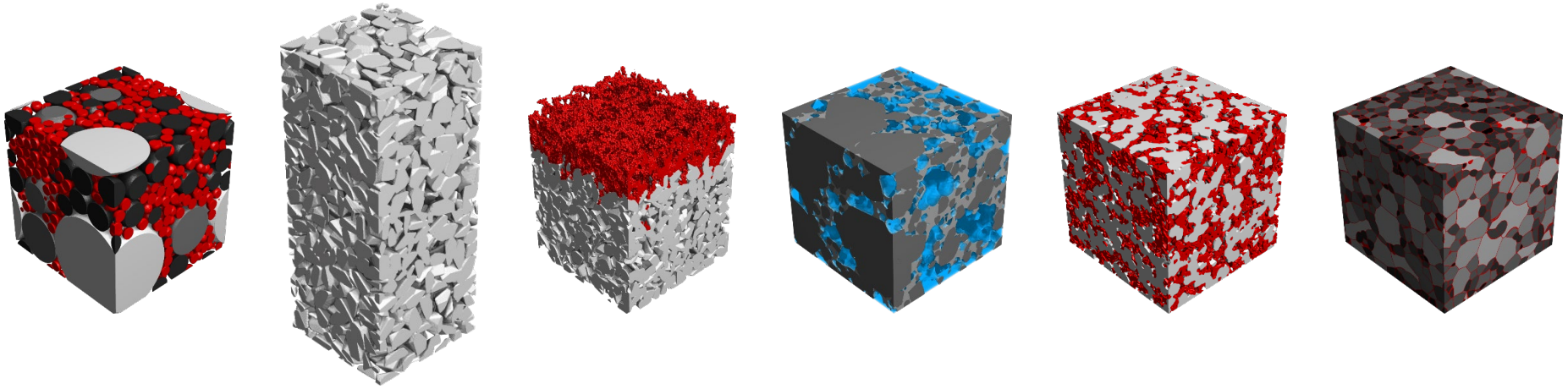
- Modelling of packed beds of spheres.
- Modelling of ceramics in different stages of sintering.
- Modelling of catalyst layer and microporous layer in PEM fuel cells.
- Modelling of lithium ion cathodes and other battery materials.
- Modelling of rocks- like sandstone.
- Modelling of sphere packings with very high packing density.



Binarized PMS images

from polished micrograph sections and modeled sintered ceramics

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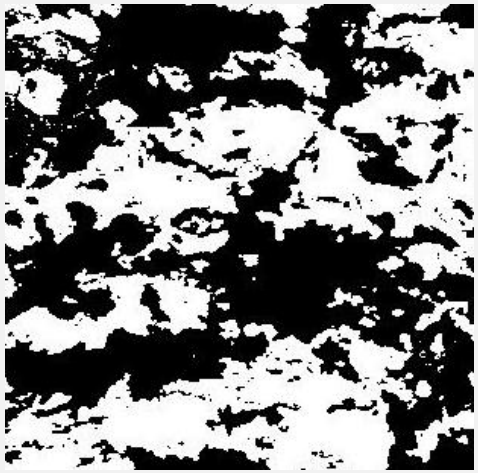
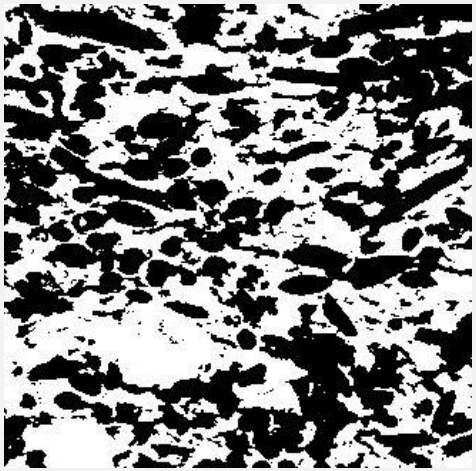
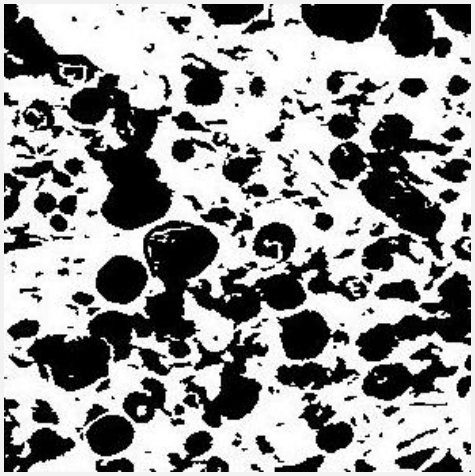
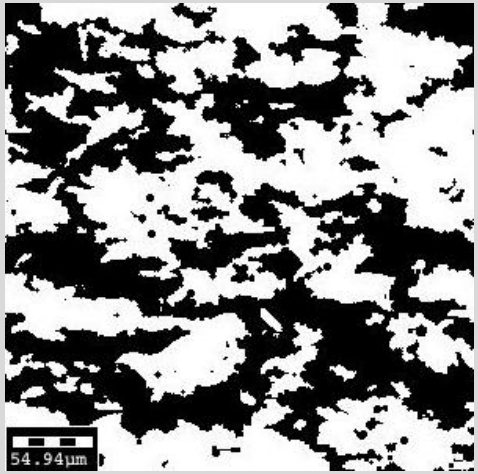
PMSs

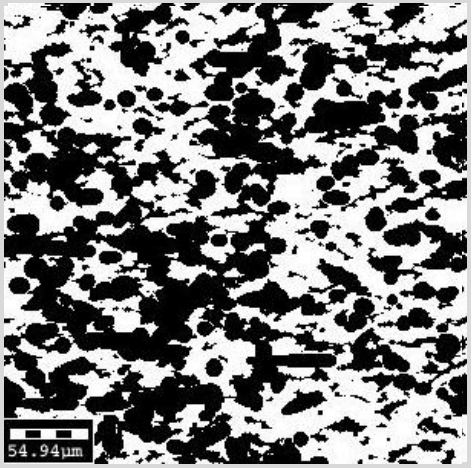


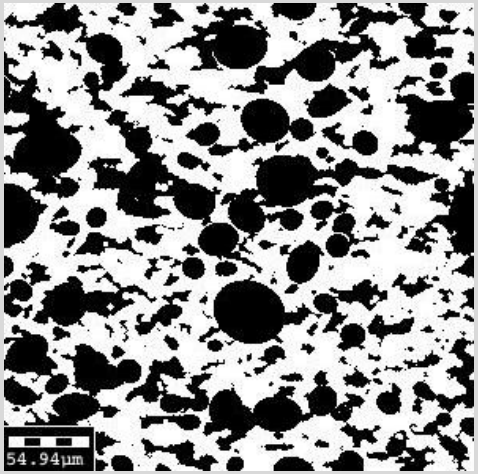




Models







CERAMIC MODEL CHARACTERIZATION

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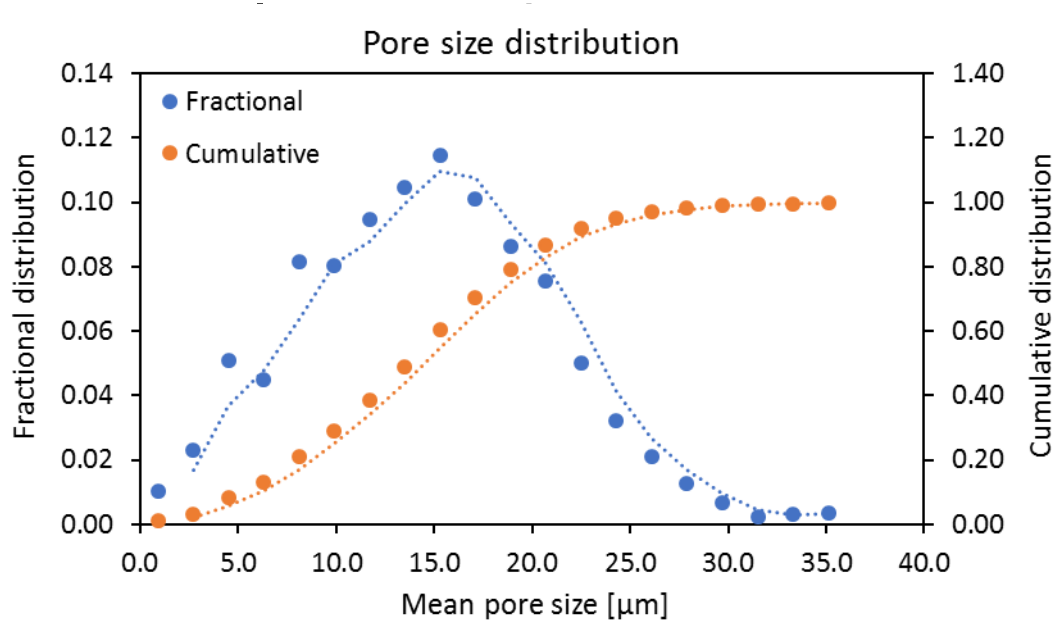
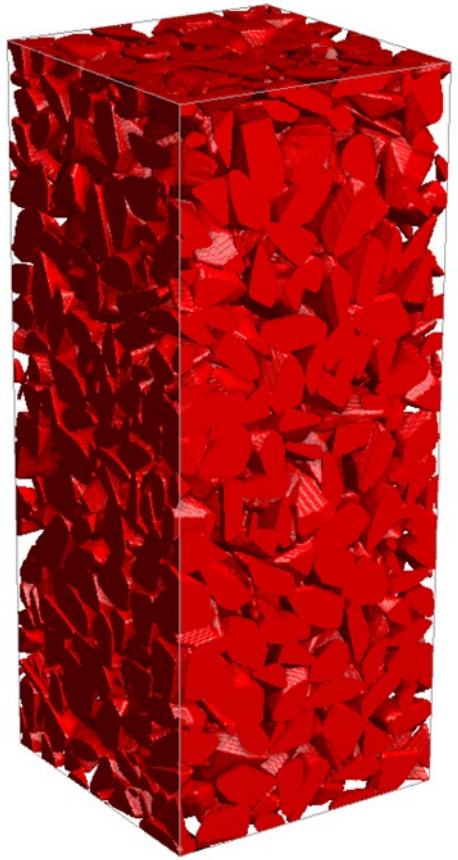
Characterizing the ceramic with PoroDict

Evaluation of the pore size distribution





CERAMIC MODEL CHARACTERIZATION

MATH
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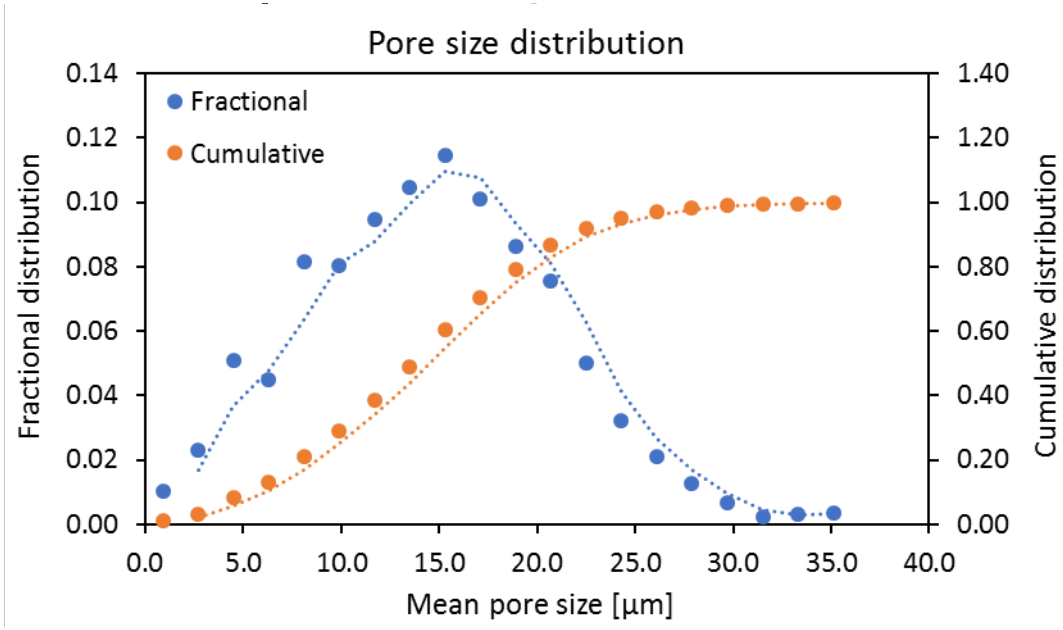

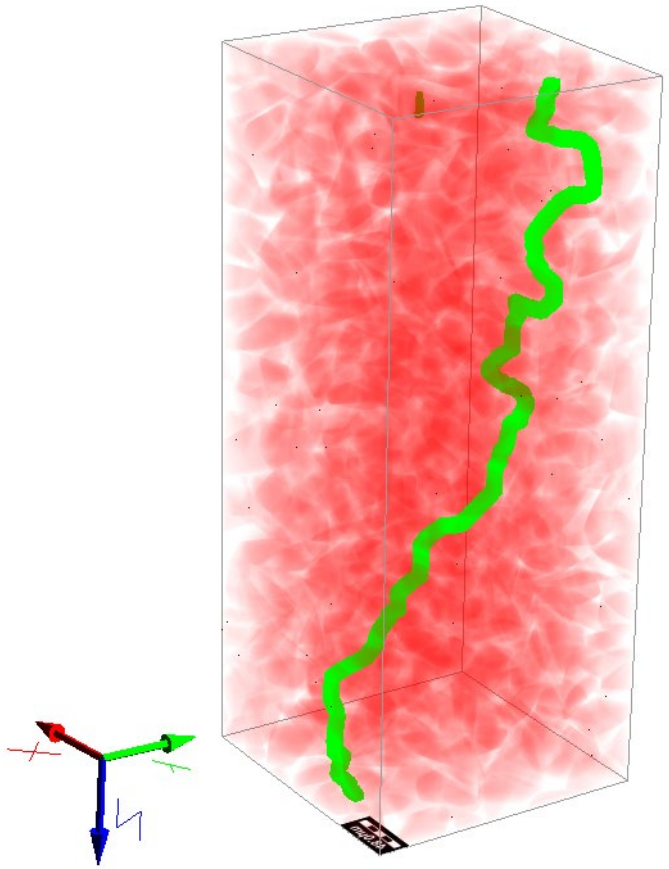

Maximum particle diameter [µm]	Path length [µm]
9.94	929.1

CERAMIC MODEL CHARACTERIZATION

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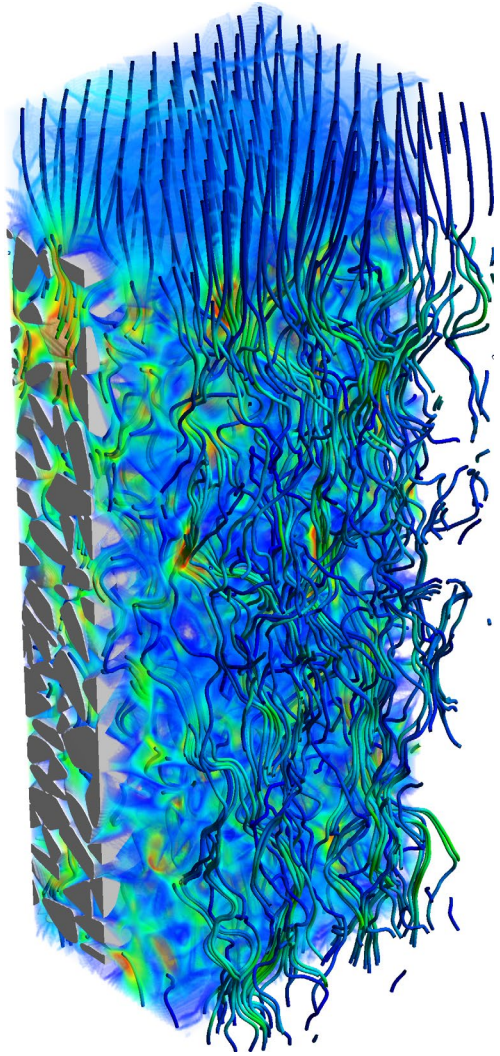
Characterizing the ceramic with FlowDict

- Domain size: 256x256x630 Voxels
- Voxel length: 0.9 µm
- Ceramic porosity: 48.7 %
- Pressure drop is 252.8 Pa at mean air flow velocity of 0.04 m/s
- Flow resistivity: 1.115e+07 kg/(m^{3}s)
- Permeability: 1.63e-12 m^2



Measured porosities & permeabilities

of real ceramics vs modeled porosities & simulated permeabilities on modeled ceramics

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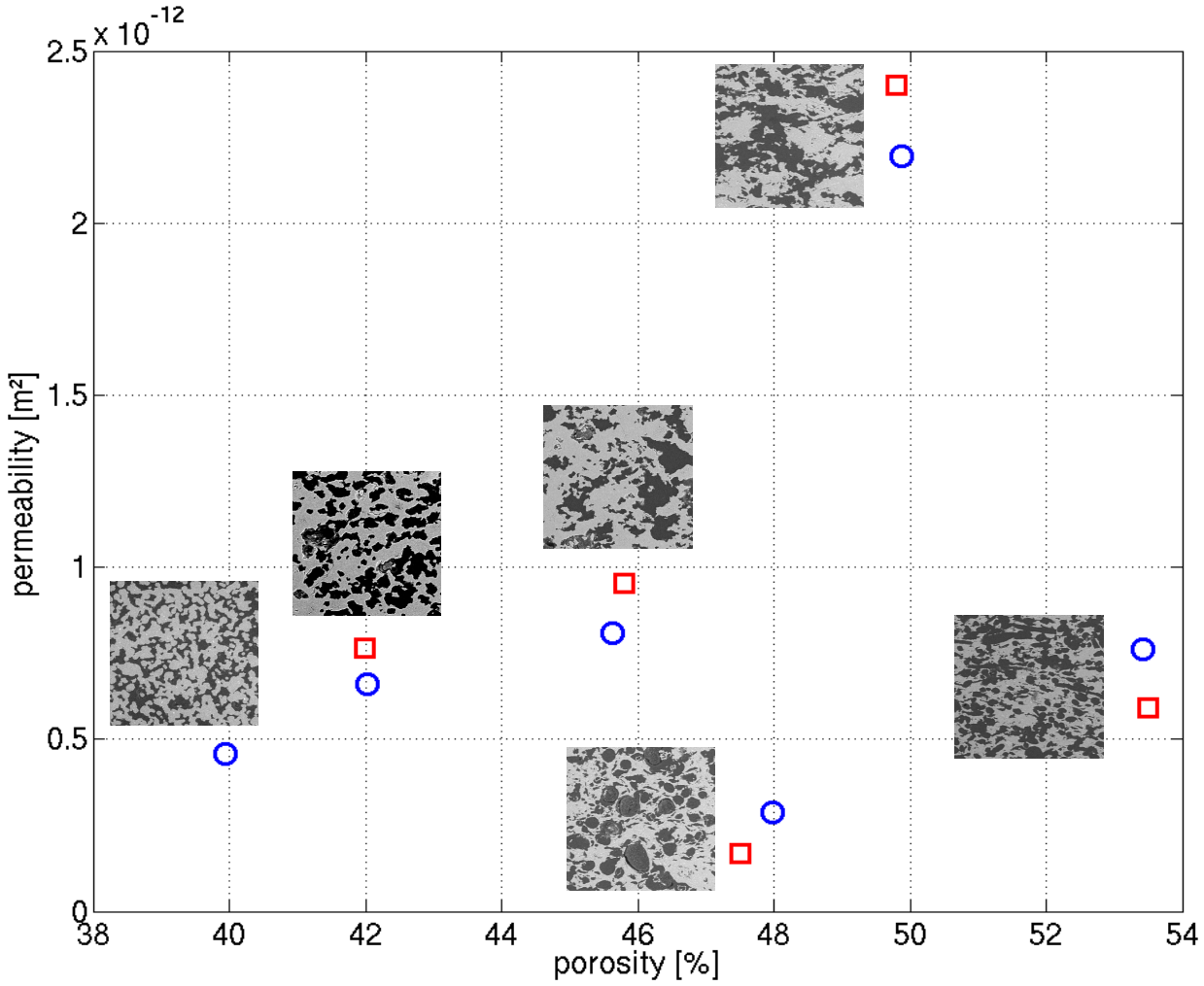

Simulation

Measurement

Filter life time simulation with FilterDict-Media

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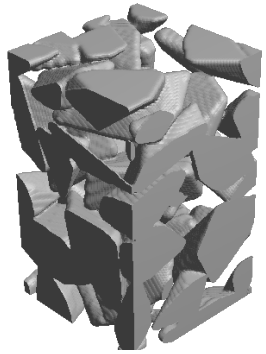
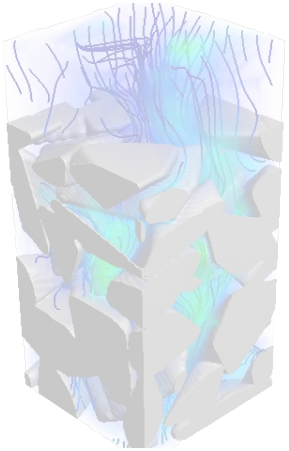
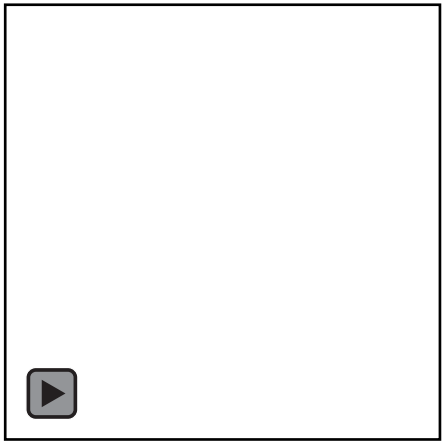


1. Model filter

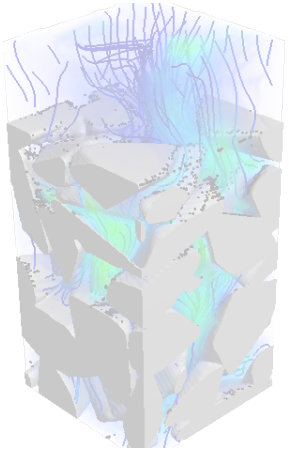


2. Compute flow field

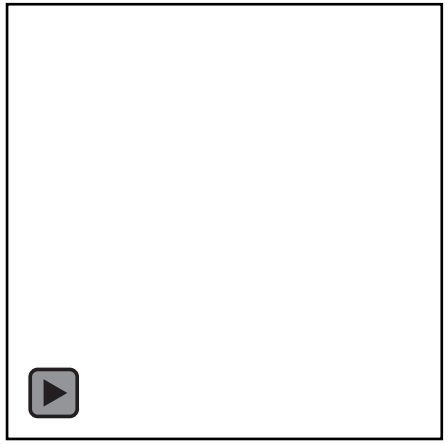


3. Track particles

4. Deposit particles



5. Update flow field



6. Repeat ...

Analysis of Cermaic Filter Performance

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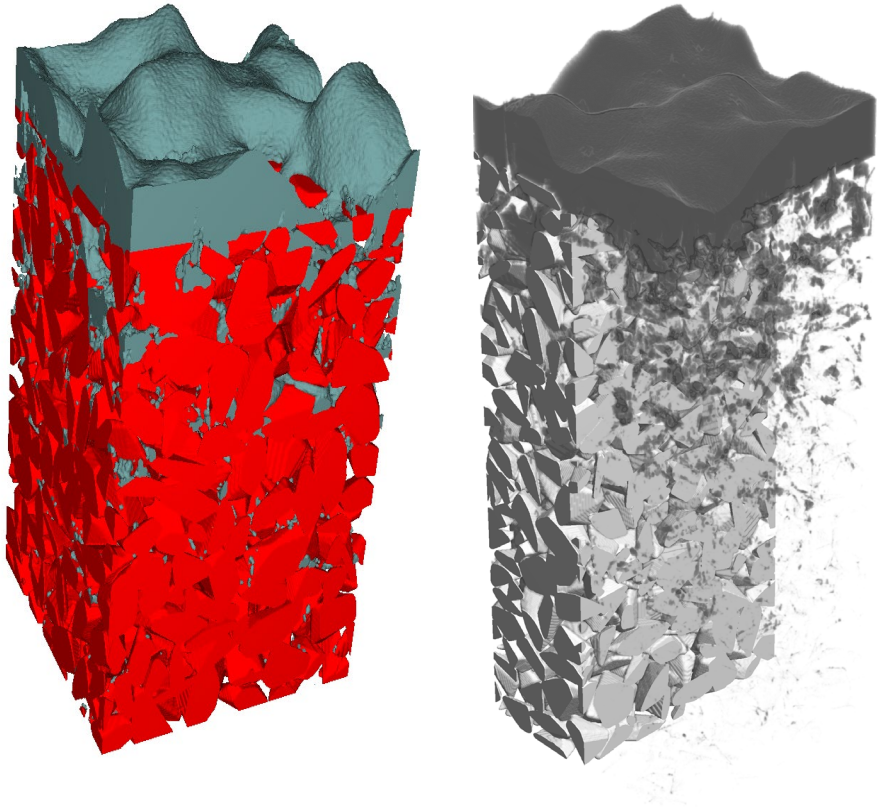
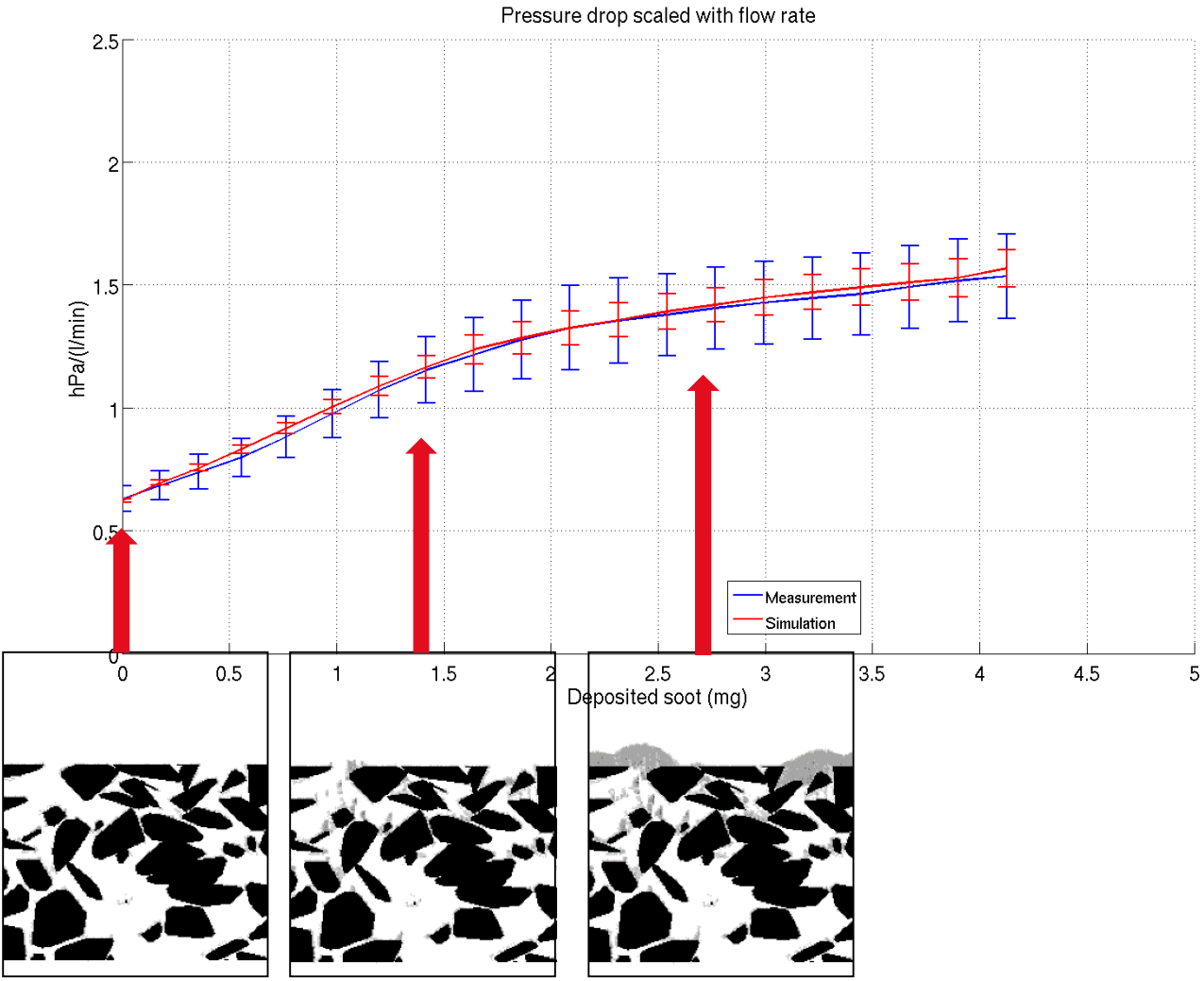
Analysis of the filtration performance with FilterDict-Media

- Simulation of soot particles deposition.
- Evaluation of fractional filter efficiency.
- Evaluation of pressure drop in depth filtration & cake filtration regimes.



Experimental and simulated pressure drop evolution



- Error bars induced by 5 measurements and 5 different realizations of the digital structure.
- Match achieved by introducing different parameters f_{max} & $\sigma(f)$ for depth & cake filtration.

L. Cheng et al., WFC 11, 2012.

Spatial particles deposition over time

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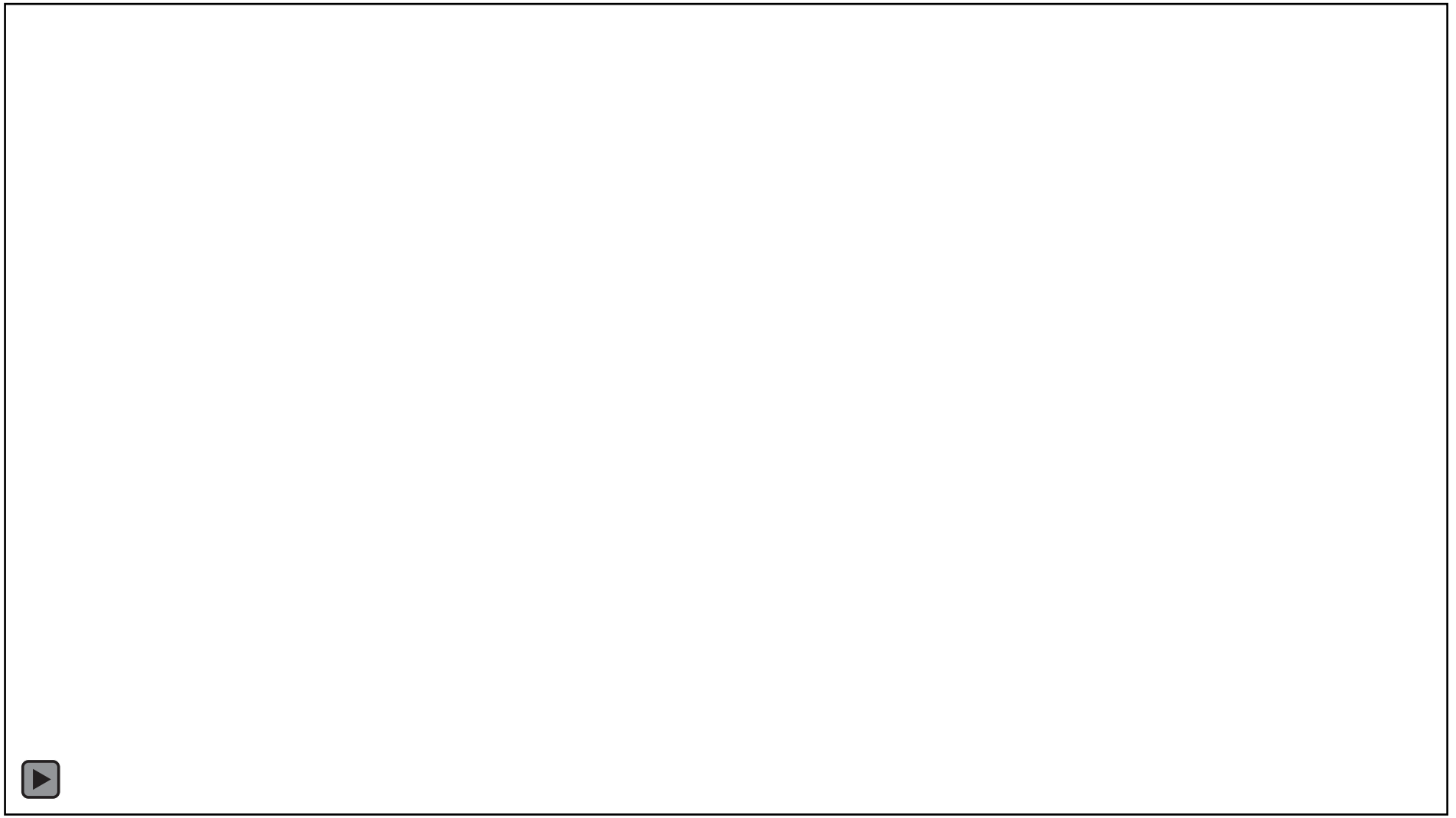

Reduced pressure drop over time

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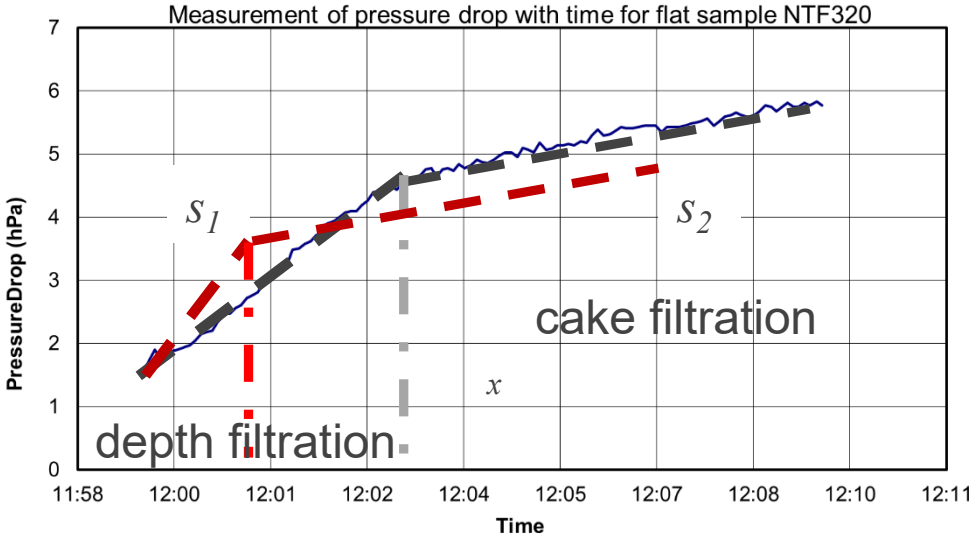
After fast initial pressure drop increase (slope s1, depth filtration phase)
follows long slower pressure drop increase (slope s2, cake filtration phase)

- Matched experiment with simulations
- **Shortened depth phase to lower pressure drop during cake phase**
- Fraunhofer IKTS manufactured ceramic, experiment matched simulations, and patent was granted: *Particulate filter, No. DE102012220181 A1*



Development of Low Pressure and High Performance GPF Catalyst

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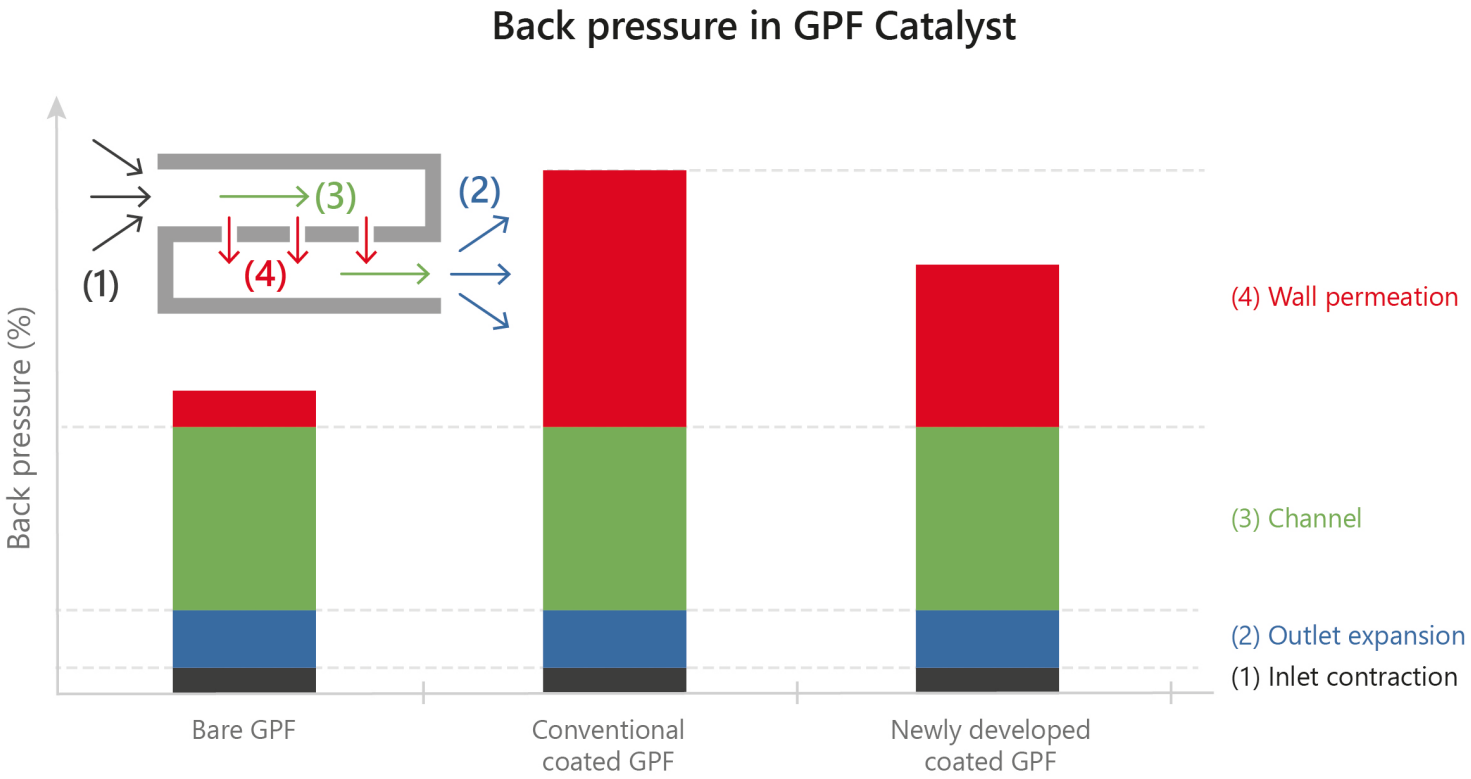

Tanaka, A., Miyoshi, N., and Sato, A., "Development of Low Pressure and High Performance GPF Catalyst," SAE Technical Paper 2018-01-1261, 2018, doi:10.4271/2018-01-1261.

Idea of the achievement: Analysis of pores in the washcoat

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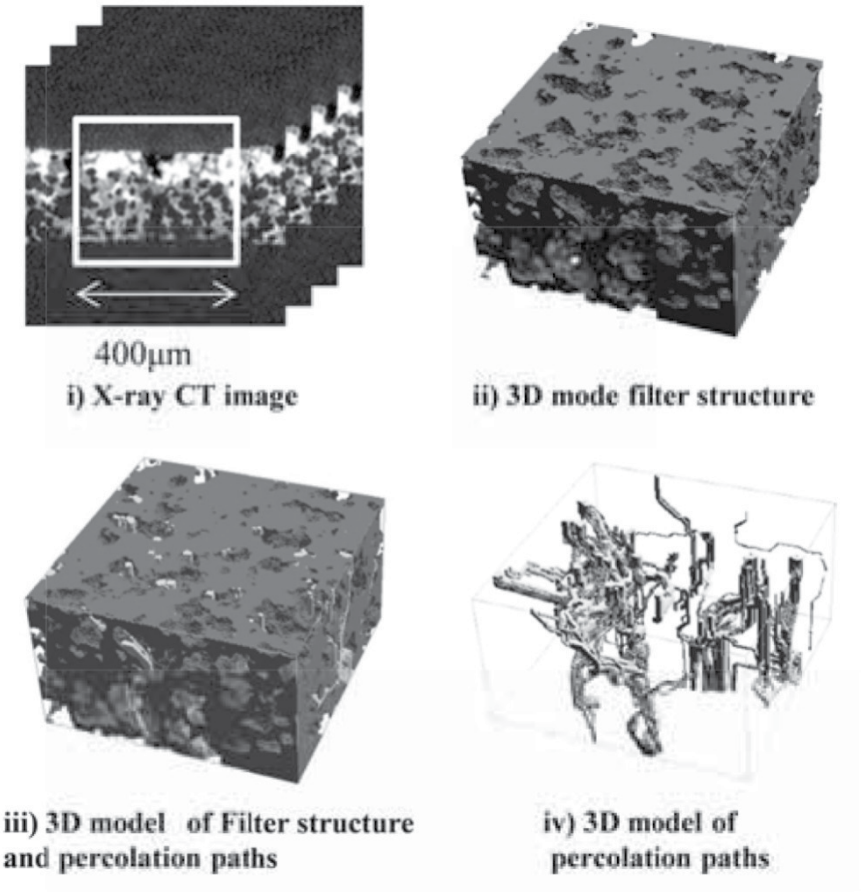

Tanaka, A., Miyoshi, N., and Sato, A., "Development of Low Pressure and High Performance GPF Catalyst," SAE Technical Paper 2018-01-1261, 2018, doi:10.4271/2018-01-1261.

PROCEDURE

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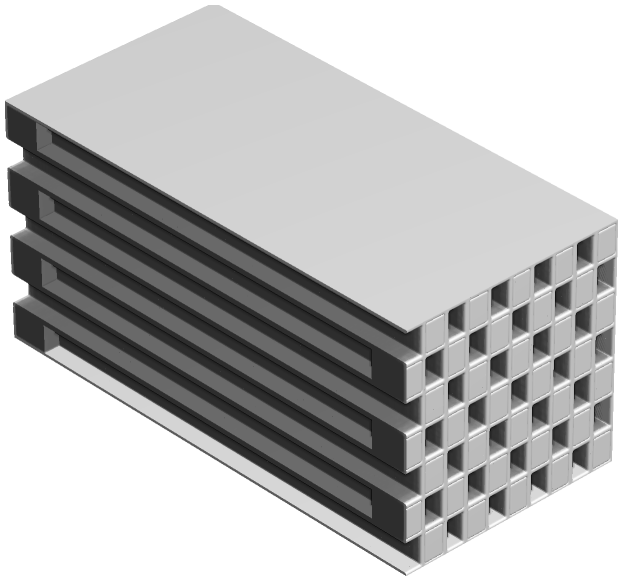
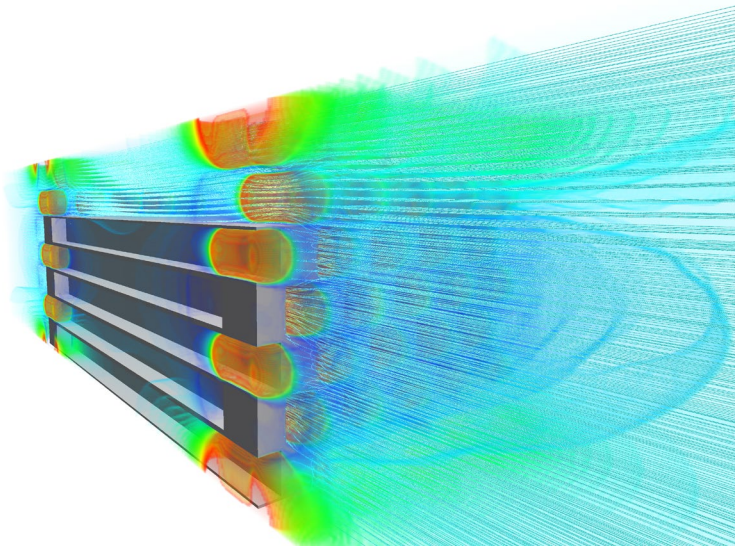
1 Simulate pressure loss across the wall

2 Simulate pressure loss along the channels





Modeling & simulation at unresolved media scale

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Using models to derive cross-property relations

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- By cross-property relations one predicts a property that is more difficult to measure by one that is easier to measure. For example, one may predict mechanical stiffness from knowledge of thermal conductivity.
- In the work with Pabst, Uhlířová and Gregorová, 3D periodic models with desired characteristics are created and the mechanical and thermal properties are computed. Cross-property shortcut formulas can thus be validated.
- Once the numerical method is established against experiments, it provides a wealth of numerical experimental data at much lower cost in time and materials than real experiments.
- It may lead to a stream of publications by the ceramic

Example: porosity study 1
Closed-cell Kelvin foams

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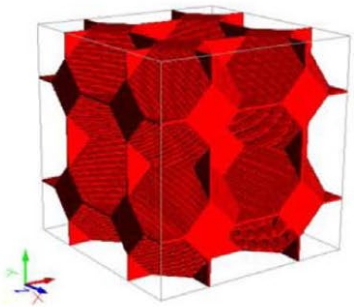
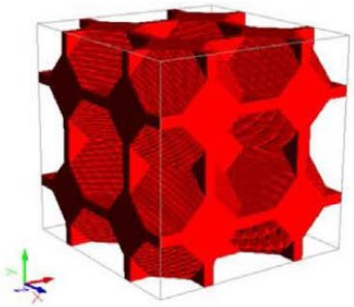
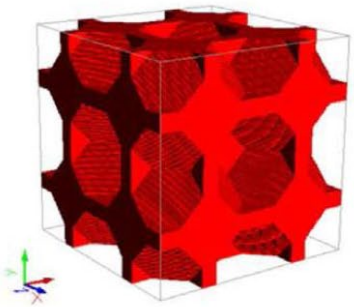
W. Pabst et al. *Journal*



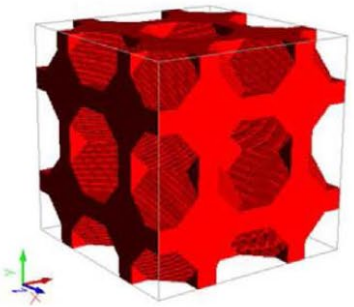
$\phi = 92.7\ \%$



$\phi = 69.3\ \%$



$\phi = 57.4\ \%$



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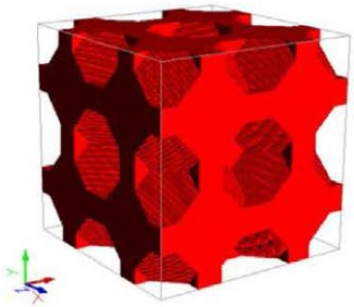
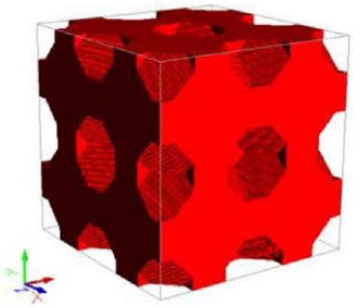
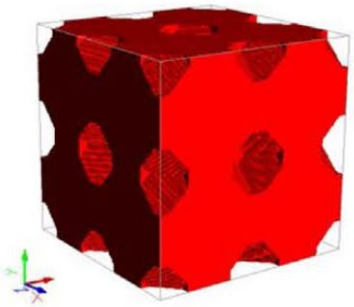


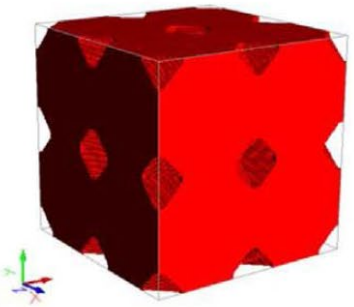
$\phi = 36.7\ \%$



$\phi = 22.7\ \%$



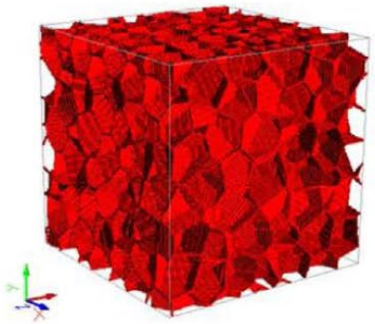
$\phi = 11.9\ \%$



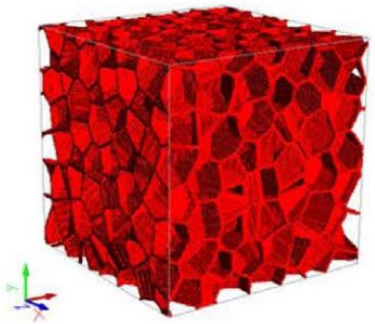
$\phi = 5.2\ \%$

Example: porosity study 2
Closed-cell random foams

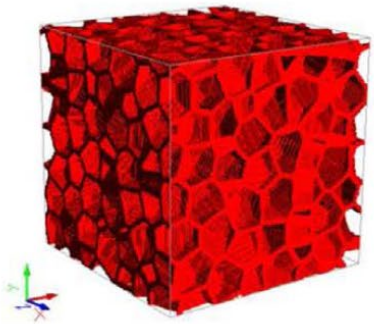
MATH
2 MARKET



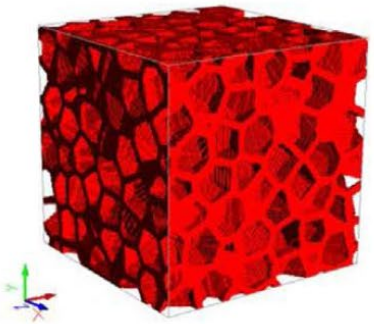
$\phi = 91.3\,\%$



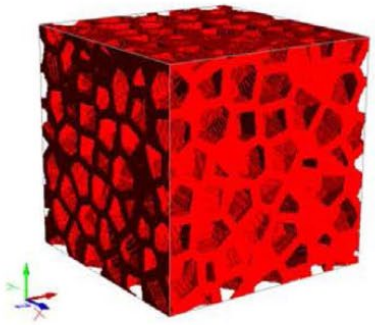
$\phi = 83.1\,\%$



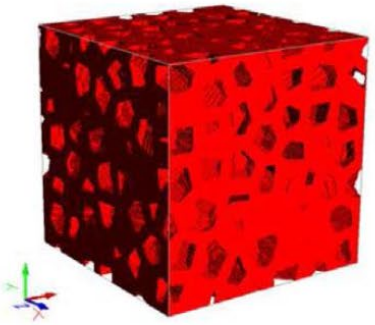
$\phi = 68.2\,\%$



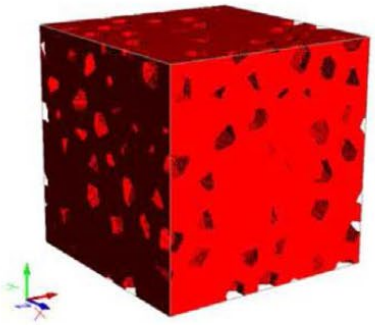
$\phi = 55.2\,\%$



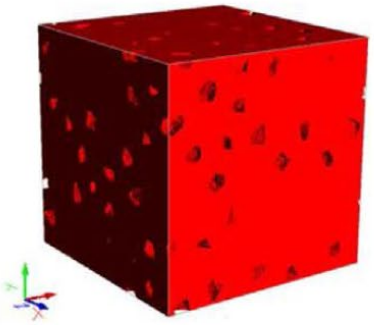
$\phi = 43.9\,\%$



$\phi = 29.9\,\%$



$\phi = 16.3\,\%$



$\phi = 6.0\,\%$

Example: porosity study 3 Kelvin-cell strut-based microstructures

MATH
2 MARKET

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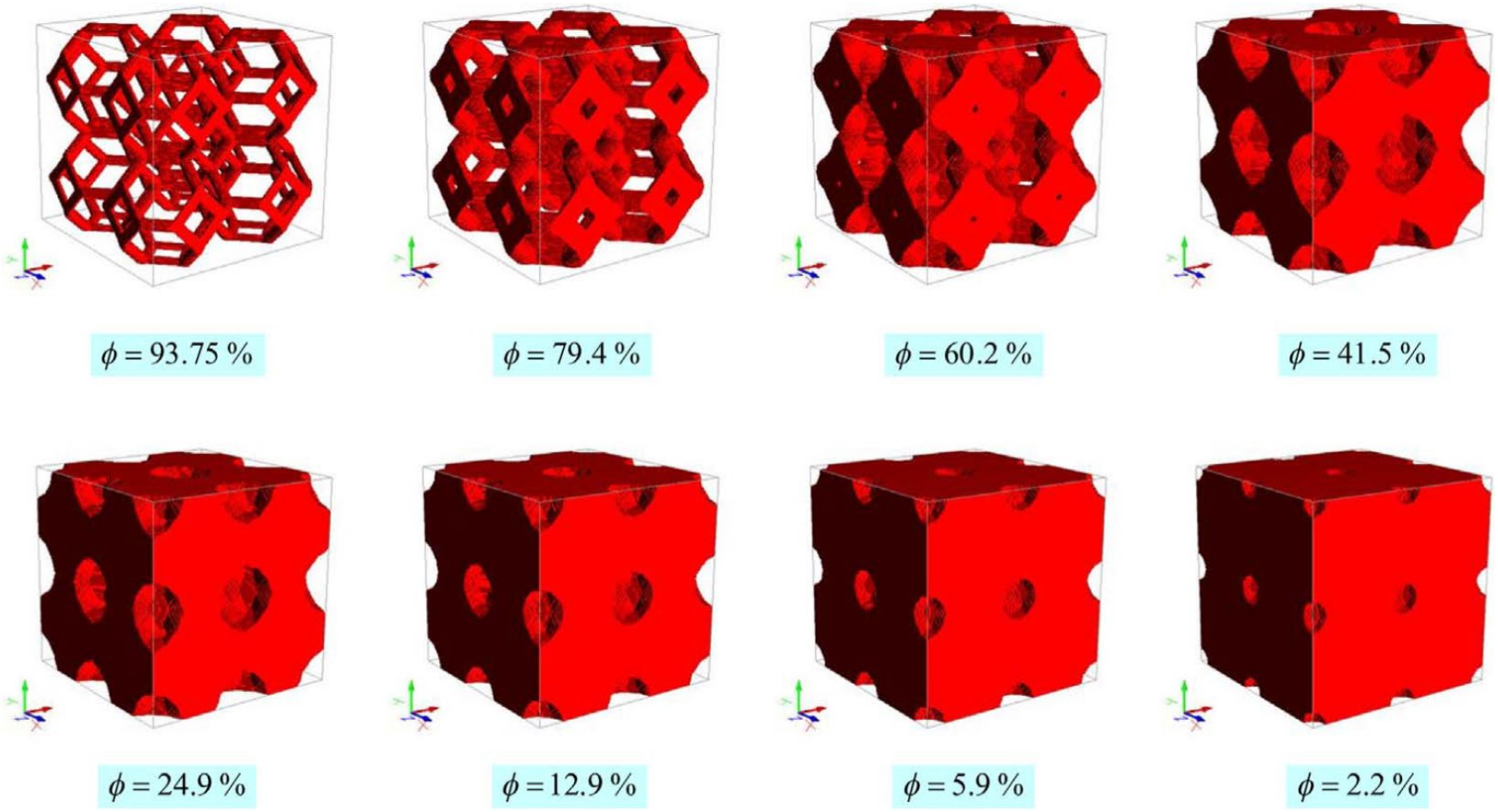
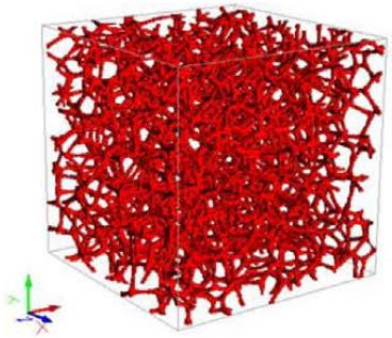
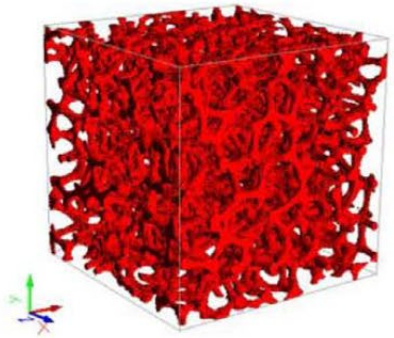


Example: porosity study 4 random Strut-based microstructures

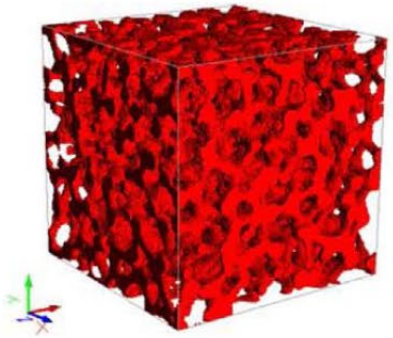
MATH 2 MARKET



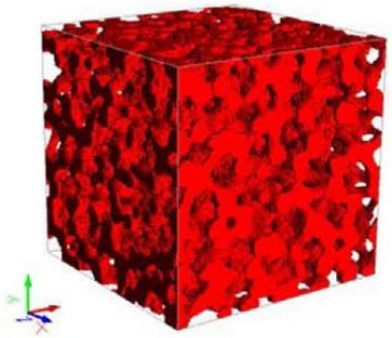
$\phi = 95.7\,\%$



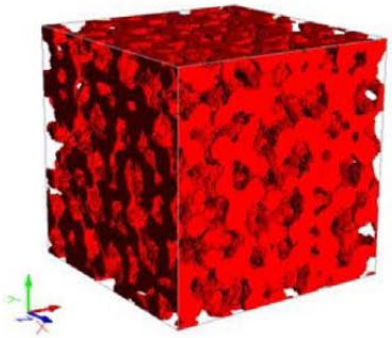
$\phi = 84.8\,\%$



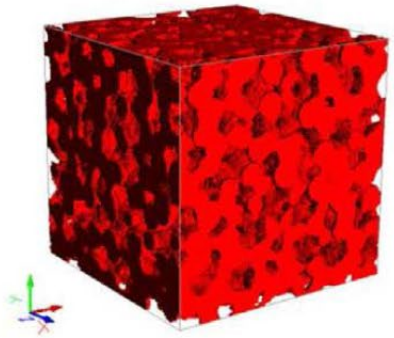
$\phi = 68.3\,\%$



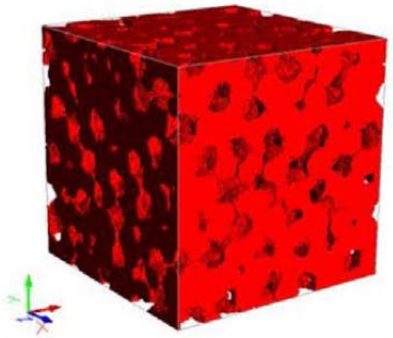
$\phi = 55.8\,\%$



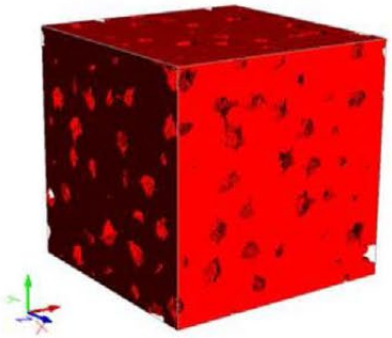
$\phi = 47.1\,\%$



$\phi = 38.5\,\%$



$\phi = 26.4\,\%$



$\phi = 11.0\,\%$

Example: porosity study 5
Inverse Kelvin Foam

MATH
2 MARKET

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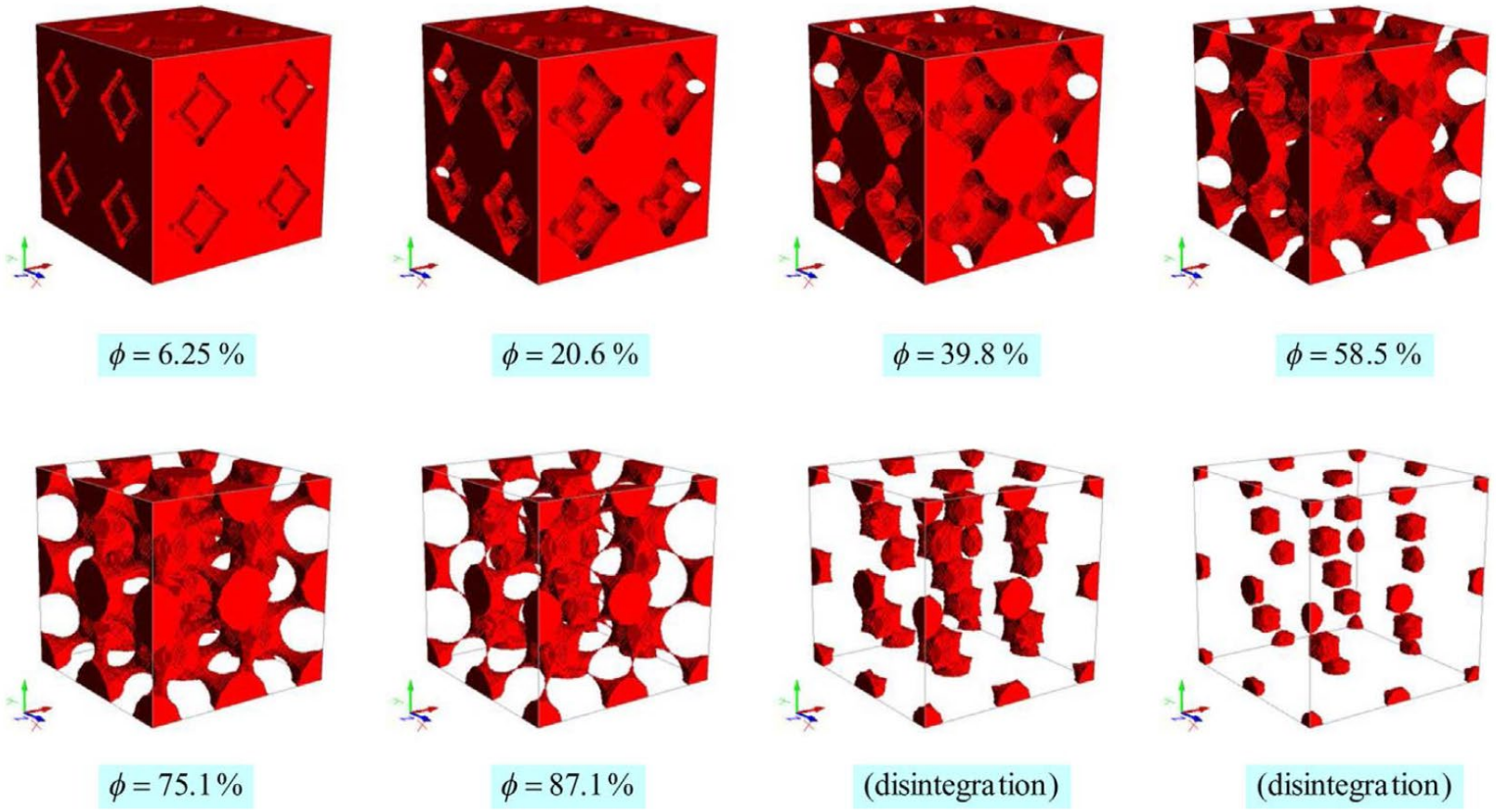
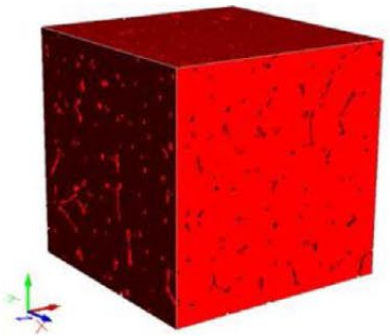
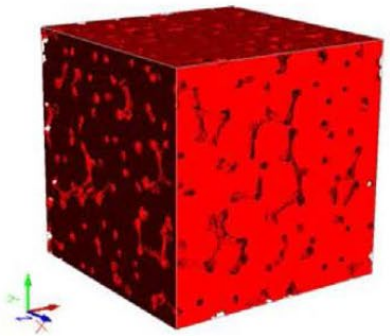


Example: porosity study 6
Random Foam

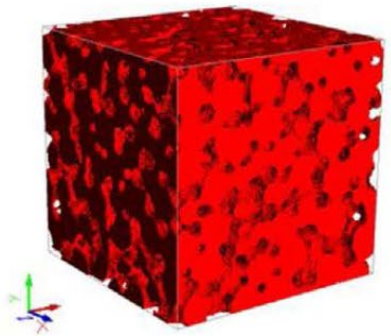
MATH
2 MARKET



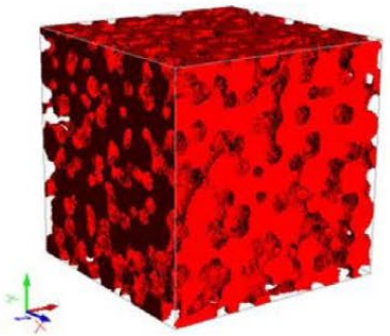
$\phi = 4.3\,\%$



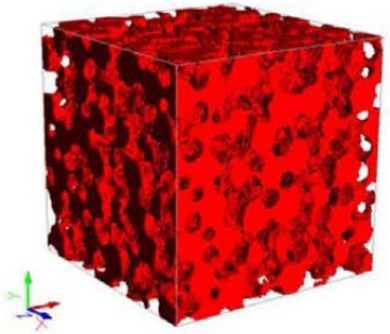
$\phi = 15.2\,\%$



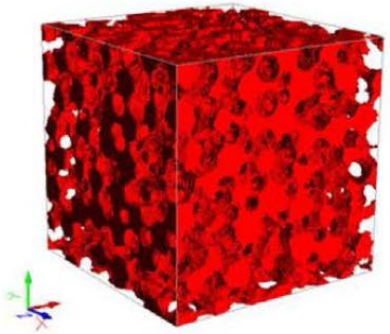
$\phi = 31.7\,\%$



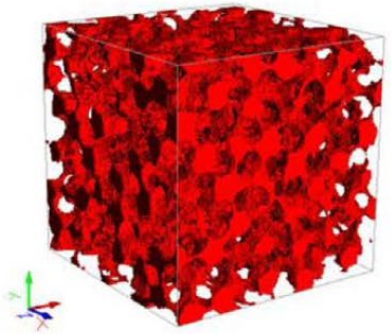
$\phi = 44.2\,\%$



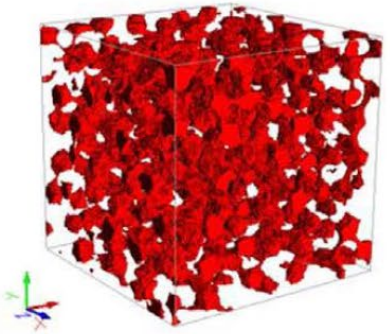
$\phi = 52.9\,\%$



$\phi = 61.5\,\%$

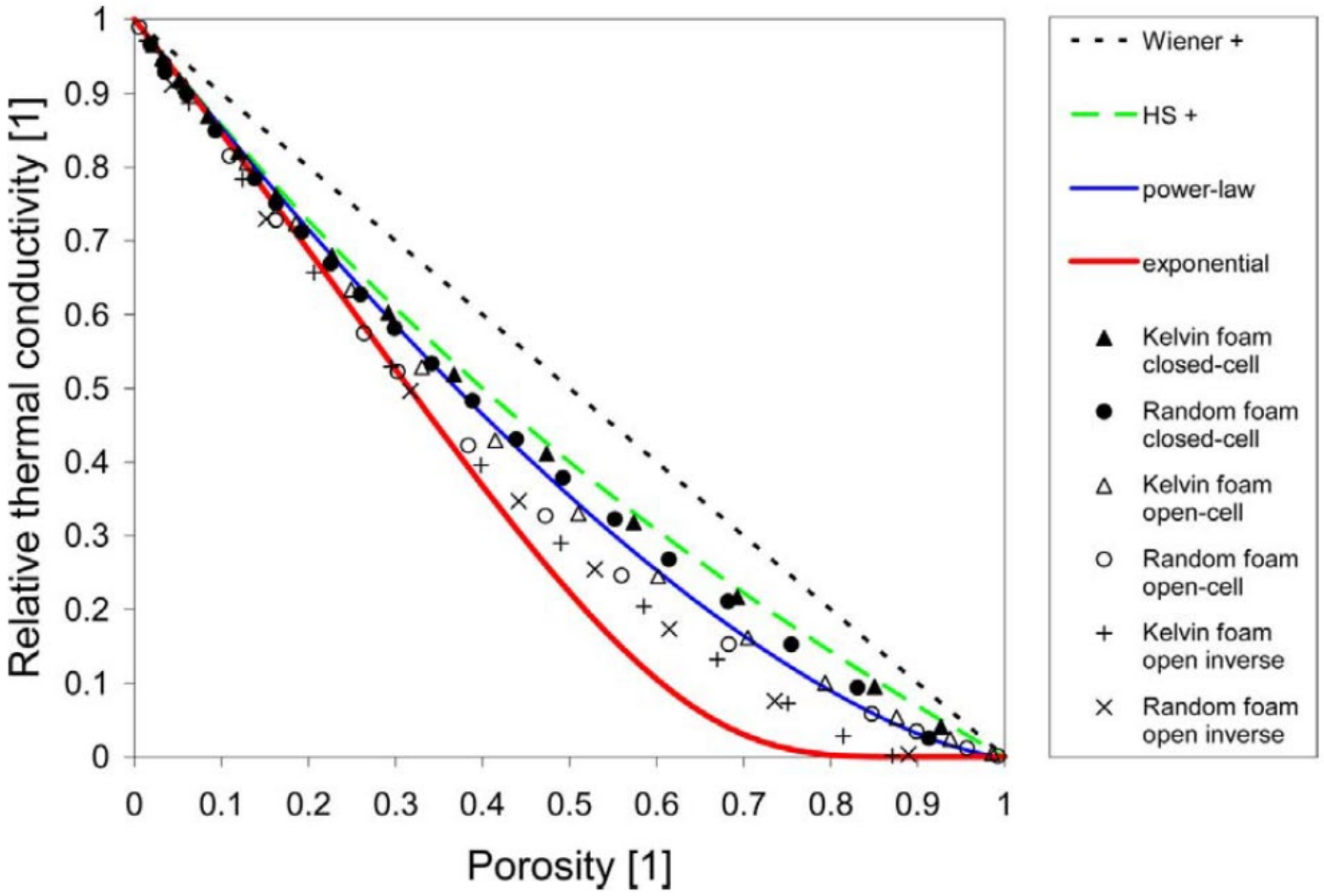


$\phi = 73.6\,\%$



$\phi = 89.0\,\%$

Simulated relative Thermal Conductivity as function of porosity



Simulated relative Young's Modulus as function of porosity

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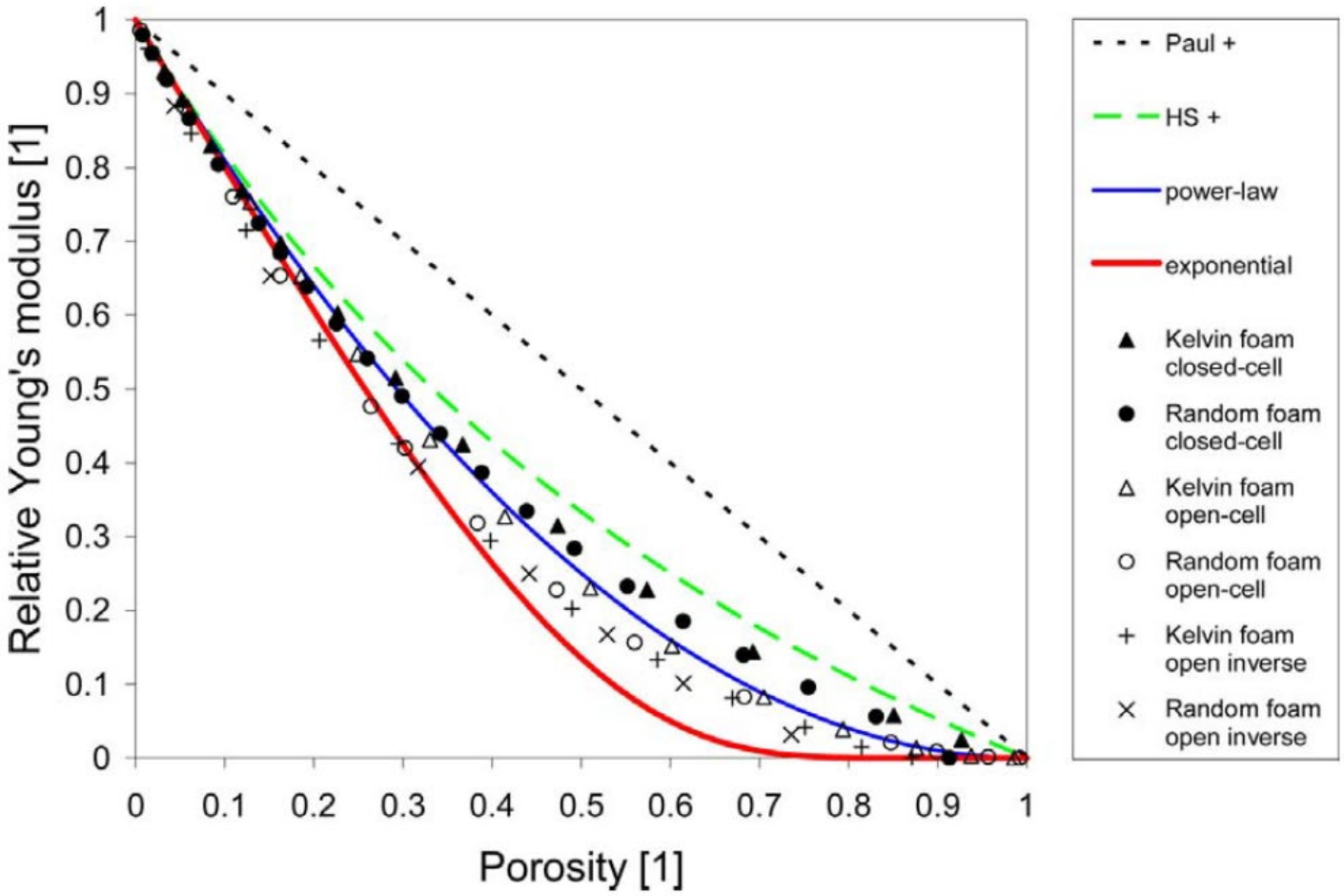
2 MARKET



PUBLICATIONS BASED ON THIS SYNERGY

MATH 2 MARKET

- Tereza Uhlířová, Willi Pabst, Conductivity and Young's modulus of porous metamaterials based on Gibson-Ashby cells, Scripta Materialia, Volume 159, **2019**, Pages 1-4, https://doi.org/10.1016/j.scriptamat.2018.09.005.
- Tereza Uhlířová, Willi Pabst, Thermal conductivity and Young's modulus of cubic-cell metamaterials, Ceramics International, Volume 45, Issue 1, **2019**, Pages 954-962, https://doi.org/10.1016/j.ceramint.2018.09.271.
- Tereza Uhlířová, Vojtěch Nečina, Willi Pabst, Modeling of Young's modulus and thermal conductivity evolution of partially sintered alumina ceramics with pore shape changes from concave to convex, Journal of the European Ceramic Society, Volume 38, Issue 8, **2018**, Pages 3004-3011, https://doi.org/10.1016/j.jeurceramsoc.2017.12.033.
- Willi Pabst, Tereza Uhlířová, Eva Gregorová, Shear and bulk moduli of isotropic porous and cellular alumina ceramics predicted from thermal conductivity via cross-property relations, Ceramics International, Volume 44, Issue 7, **2018**, Pages 8100-8108, https://doi.org/10.1016/j.ceramint.2018.01.254.
- Willi Pabst, Tereza Uhlířová, Eva Gregorová, Andreas Wiegmann, Relative Young's modulus and thermal conductivity of isotropic porous ceramics with randomly oriented spheroidal pores – Model-based relations, cross-property predictions and numerical calculations, Journal of the European Ceramic Society, Volume 38, Issue 11, **2018**, Pages 4026-4034, https://doi.org/10.1016/j.jeurceramsoc.2018.04.051.
- Willi Pabst, Tereza Uhlířová, Eva Gregorová, Andreas Wiegmann, Young's modulus and thermal conductivity of closed-cell, open-cell and inverse ceramic foams – model-based predictions, cross-property predictions and numerical calculations, Journal of the European Ceramic Society, Volume 38, Issue 6, **2018**, Pages 2570-2578,, https://doi.org/10.1016/j.jeurceramsoc.2018.01.019.
- Willi Pabst, Tereza Uhlířová, Eva Gregorová, Andreas Wiegmann, Young's modulus and thermal conductivity of model materials with convex or concave pores – from analytical predictions to numerical results, Journal of the European Ceramic Society, Volume 38, Issue 7, **2018**, Pages 2694-2707, https://doi.org/10.1016/j.jeurceramsoc.2018.01.040.

Conclusion & Outlook for ceramics

MATH 2 MARKET

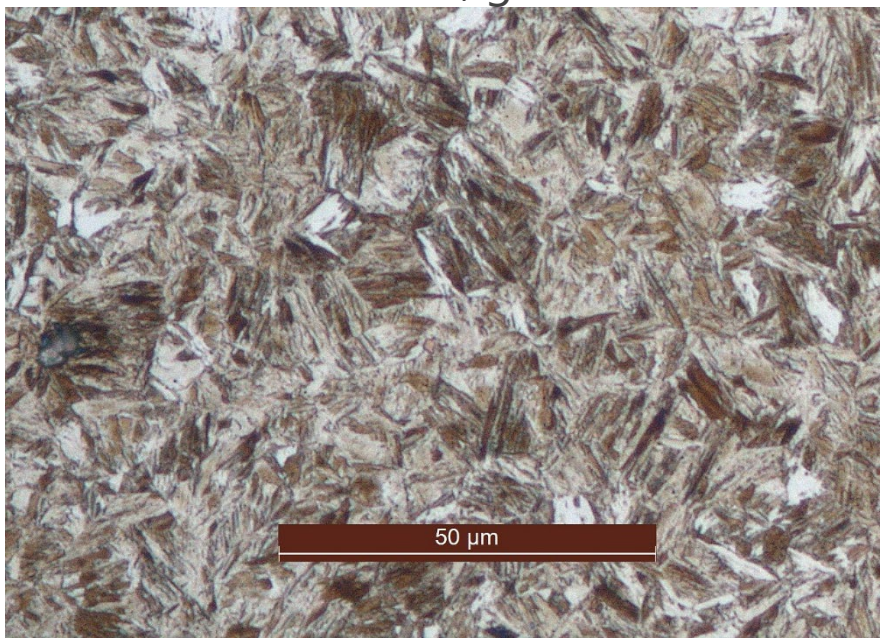
- In the knowledgeable hands of ceramics researchers, modelling and simulating properties takes only minutes
  - And complete studies can be conducted using far less time and money than real studies would
  - In the case of the previous slides, relationships between thermal conductivity and Young's modulus can be refuted and confirmed.
- Maybe other questions can be studied on ceramic models than cross-property-relations?
  - Modelling of sub-structures
  - Large deformations of ceramics
  - Mineral dissolution and precipitation in ceramics
  - Influence of radiation on effective thermal conductivity

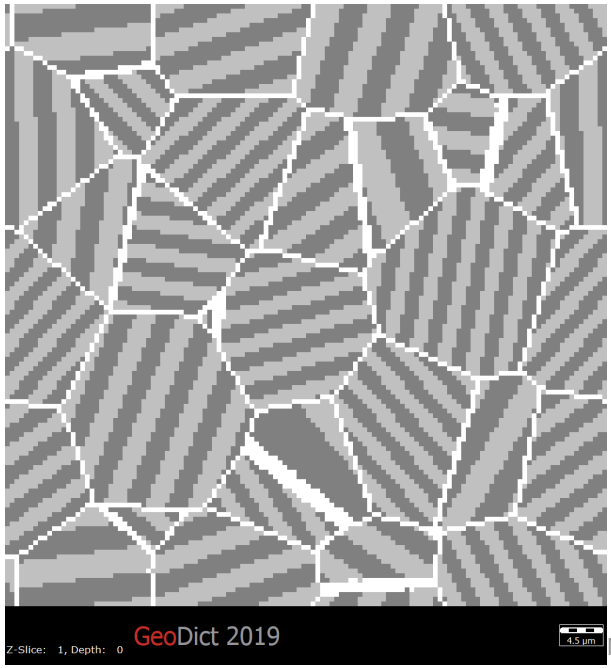
Modelling of Martensite

MATH
2 MARKET

- Martensite is formed when faced centered austenite is quenched and transforms into a highly strained body-centered tetragonal form.
- The remaining austenite and the martensite have different mechanical properties

  → Properties of microstructure can be simulated.
- Martensite is available in GrainGeo.
- In GeoDict 2020, grain orientations can be defined in the GUI.

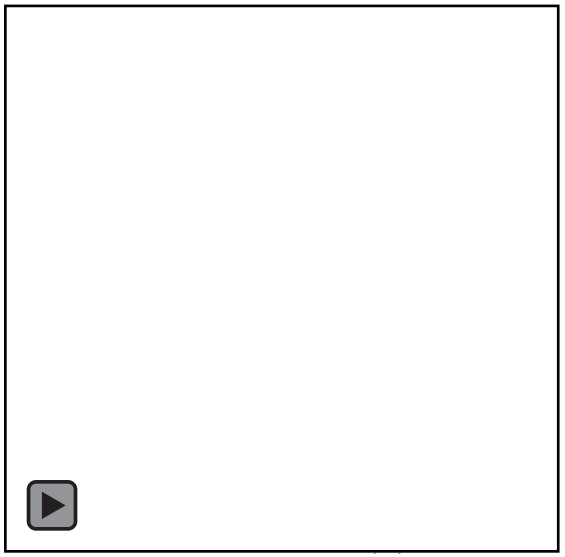


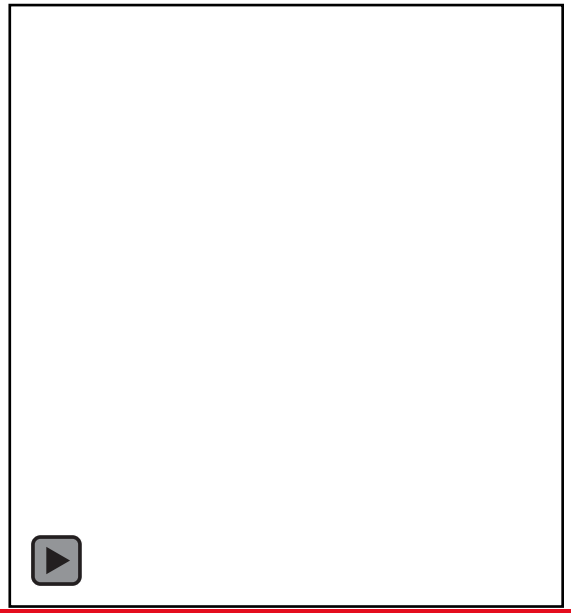


Compression of Generated Foams

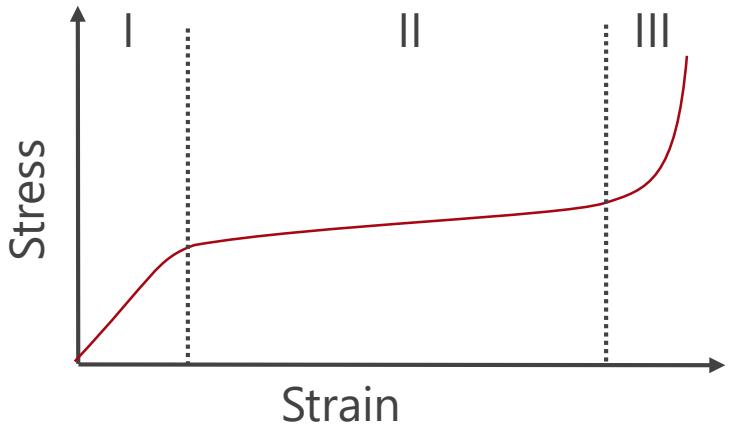
MATH 2 MARKET

Stress-strain curve calculated with GeoDict





Theoretical stress strain curve



I. Linear elasticity,
II. Plateau
III. Densification

- Foam generated with FoamGeo
- 80 % compression (on deformed geometry)
- Buckling of cell walls can be observed
- Characteristic stress strain curve
- Constant positive pore pressure

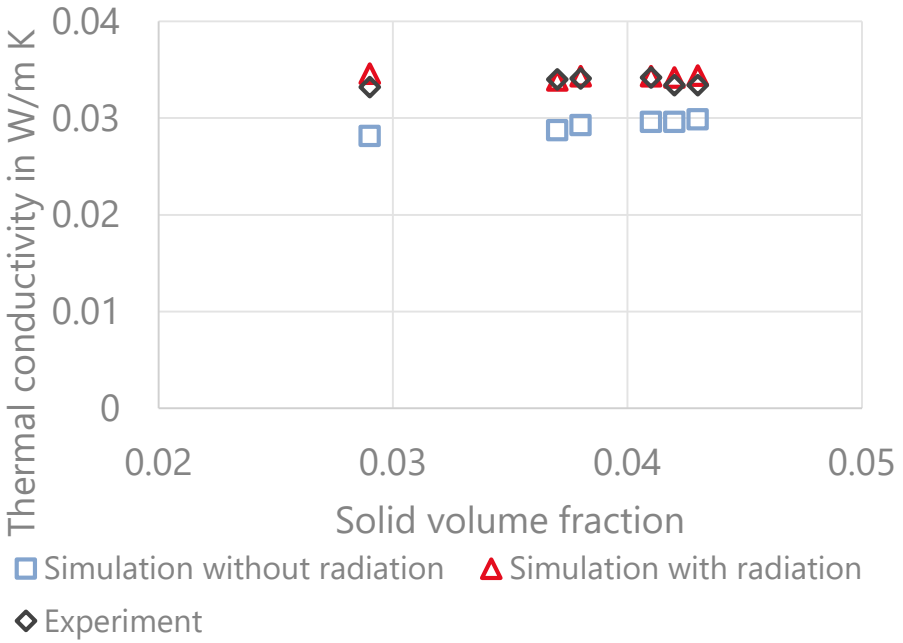
Comparison to Experiment

MATH 2 MARKET

Scope: Determination of thermal conductivity of foams and comparison to experimental data[1]

Input: Solid volume fraction of open cell polyurethane (PU) foam, physical properties of PU and air

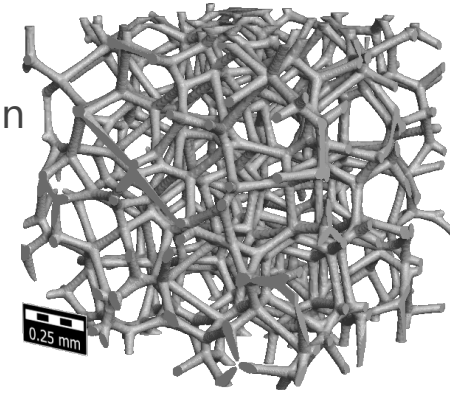
Result: Good compliance with experiments if radiation is taken into account



Thermal conductivity by radiation k_{rd}[2]:

$$k_{rd} = \frac{16 \cdot \sigma \cdot T_m^3}{3(42.038 \rho_{PU} V_f + 121.55)}$$

σ: Stefan-Boltzmann constant
T_m : mean temperature
ρ_{PU}: density of PU
V_f: solid volume fraction

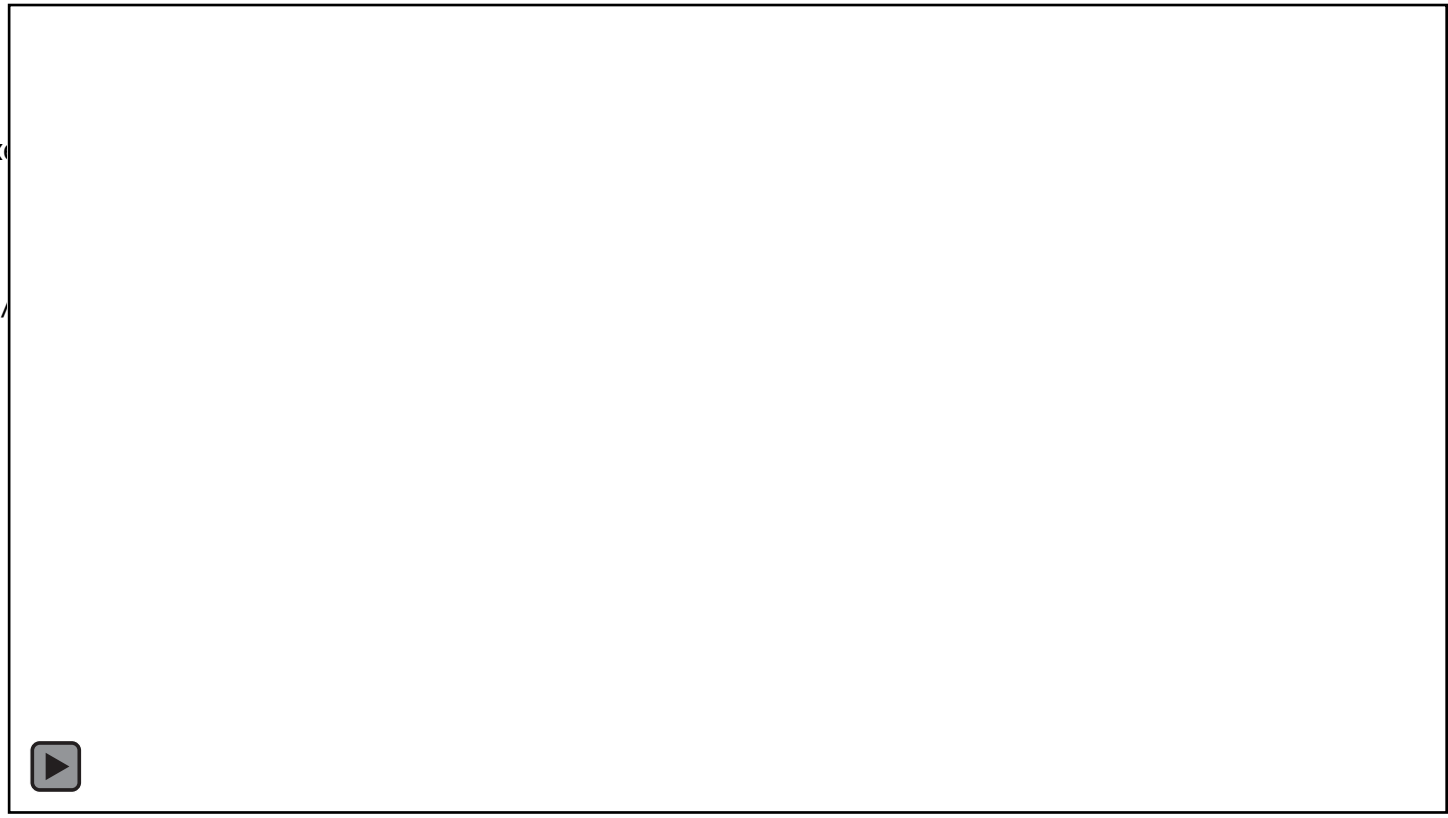


[1] J-W. Wu et al.. (1999) Thermal conductivity of polyurethane foams. *Int. J. Heat Mass Transfer,* 42, 2211-2217
[2] Tao, W.-H., Hsu, H.-C., Chang, C.-C., Hsu, C.-L., & Lin, Y.-S. (2001). Measurement and Prediction of Thermal Conductivity of Open Cell Rigid Polyurethane Foam. *Journal of Cellular Plastics*, *37*(4), 310–332.

Simulation of mineral dissolution of a rock

MATH 2 MARKET

Simulation settings:
Domain: 1024x1024x1280 voxe
Average velocity: 0.01 m/s
pH value: 2.5
Simulation time: 250 s
Number of particles: ~60.000 /



What have you seen?

MATH
2 MARKET

- Microstructure simulation software by mathematicians, physicists and computer scientists can be used to
  - Create patent for DPF (with Fraunhofer IKTS)
  - Create new washcoat for TWC (with Toyota Motor Comp)
  - Create relevant publications (with Prague University)
- Do many more things that wait to be exploited for ceramic materials
  - Large deformations
  - Internal structures
  - Radiation
  - Dissolution / precipitation
  - Etc. etc.

Thank You for your Attention

MATH
2 MARKET