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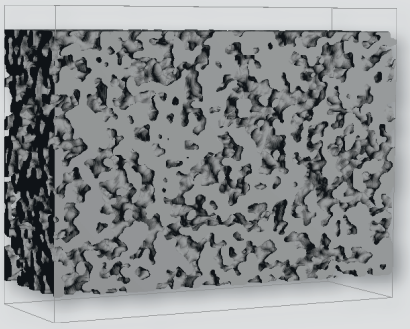
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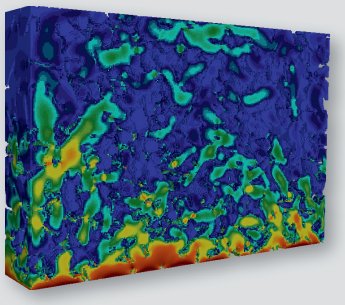
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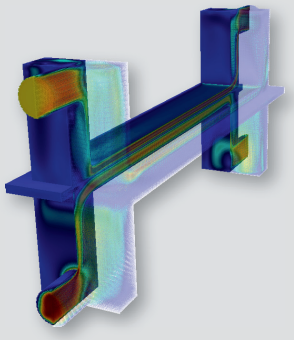
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PoreChem

SIMULATION OF REACTIVE TRANSPORT IN FILTRATION AND PURIFICATION

Assisting you in designing and selecting proper filtering media for your application

Reactive transport in porous materials like filter media for functionalized membranes plays a major role in many environmental and industrial applications, such as filtration, separation and catalysis, but also in oil recovery or osmosis. The interplay between the microscopic morphology of the medium and the flow and chemical characteristics makes designing these media complex and expensive, since local and microscopic conditions can have a large impact on the overall efficiency of the medium, leading to a large number of experiments being needed in the design process.

Therefore, Fraunhofer ITWM has developed **PoreChem**, which can simulate flow, surface and volumetric reactions, adsorption/desorption at pore scale. Also, osmotic processes can be simulated at pore scale and at lab scale. Thus, PoreChem allows to better understand the filtration and separation processes by performing computational experiments, reducing the number of expensive and time-consuming lab experiments dramatically.

In particular, PoreChem simulations can help in:

- Selecting best filtering media for your application.
- Design of optimized filtering media for selected application, or for a range of applications by virtual material design.
- Optimize operational parameters for the filtration, purification or osmosis setup.

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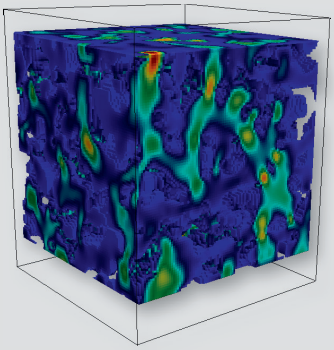

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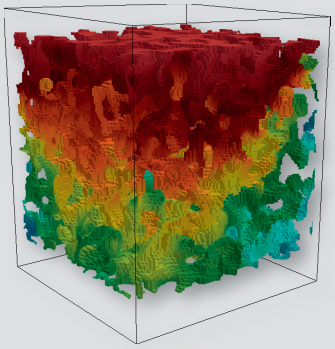

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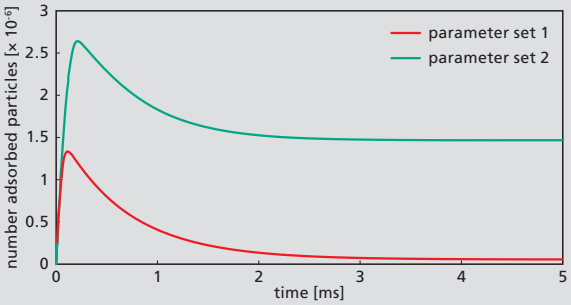

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PoreChem has been tested in a number of different applications.

Functionalized membranes

PoreChem was successfully applied to simulate the filtration of drugs from wastewater in the EU project NanoPur. In the study, a virtual representation of a real filtration membrane was generated, and then the filtration efficiency was computed with PoreChem using the surface reaction functionality (fig. 4/5). Then, parametric studies were performed to show possible improvements through alteration of the membranes morphology (fig. 6).

Osmosis

For the optimization of membranes w. r. t. forward osmosis in an experimental desalination process, the membranes were modeled from SEM images (fig. 1). Then the concentration polarization around the membrane was simulated using PoreChems osmosis functionality (fig. 2). Simulations were run, to investigate the dependence of the membrane efficiency w. r. t. the flow setup as well as membrane microstructure (fig. 3).

Further areas of applications include

- Reactive flow in catalytic converters
- Active carbon air and liquid filters
- Filtration with surface activated non-woven, woven, ceramic etc. media

PoreChem features in summary

- Three-dimensional simulation of reactive transport in complex geometries from volume data
- Simulation of kinetic and equilibrium reactions in the fluid
- Simulation of adsorption and desorption processes
- Simulation of changing computational domains through dissolution and precipitation

Services

We can assist you in the development of new and improved filter membranes in every step of the design process, from research and optimization to testing prototypes.

- Filter media characterization:
  Aquiring and processing microCT-Images for morphology characterization and generation of virtual representative microstructures.
- Consulting:
  Consulting in modeling physical and chemical processes, as well as performing simulation studies, analyzing the result and suggesting improvements to designs and control parameters.

1 *Morphology of computer generated membrane used in water purification*

2 *Pore scale flow velocity for a membrane for forward osmosis*

3 *Simulation results for flow in a lab cell element for forward osmosis*

4 *Flow through a sample of a surface activated filter membrane*

5 *Surface concentration of a reactive species*

6 *Change of the number of absorbed particles over time for two simulations*