Prediction of adsorption and break through curves by numerical simulations

E. Glatt and A. Wiegmann

Fraunhofer ITWM, Kaiserslautern, Germany

Email: glatt@itwm.fhg.de

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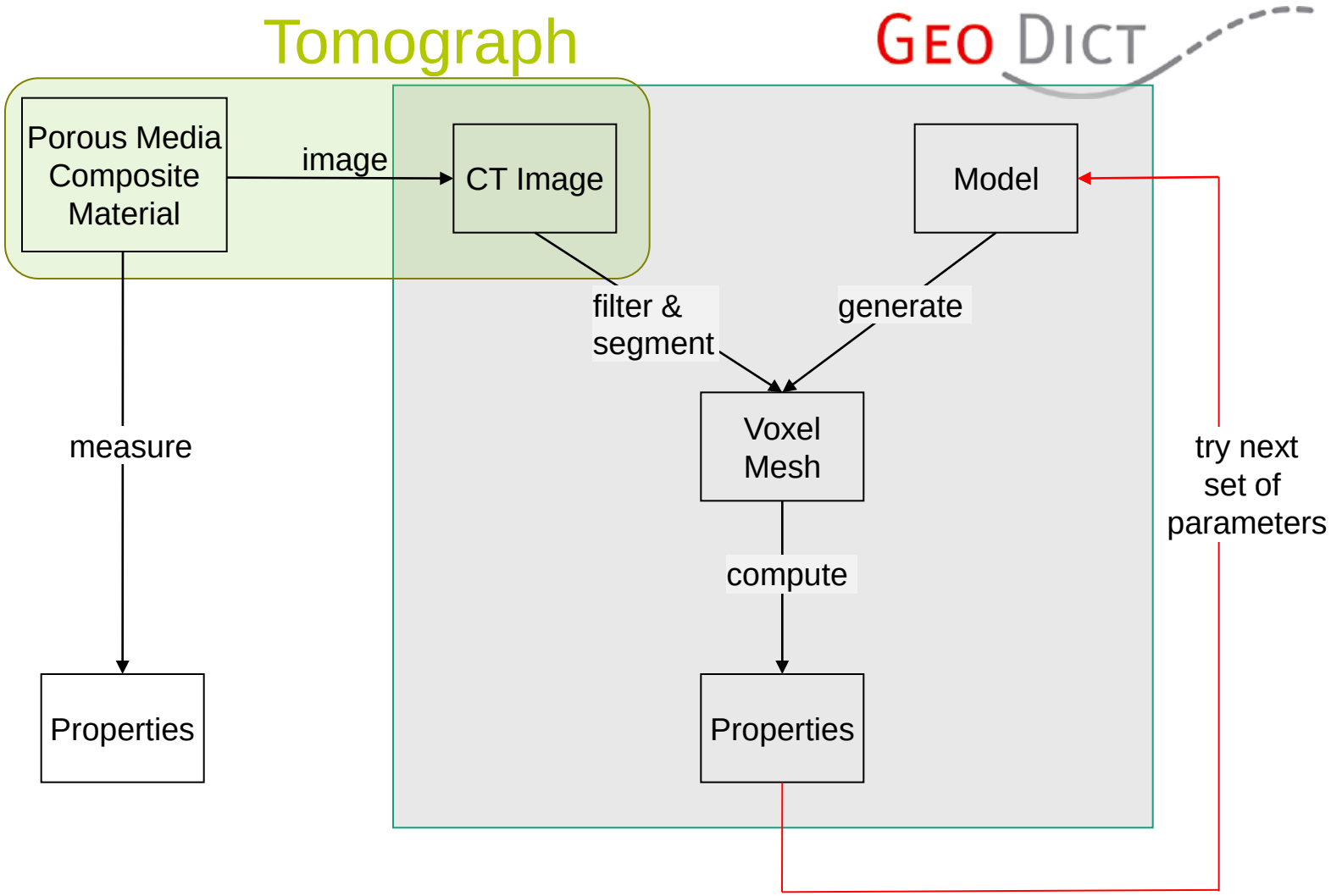
Outline

Compute Material Properties with GeoDict

CT of a granite fracture: simulation of breakthrough curves
comparison with experiment

model of a charcoal water filter: simulation of surface adsorption (case study)

Compute Material Properties with GeoDict



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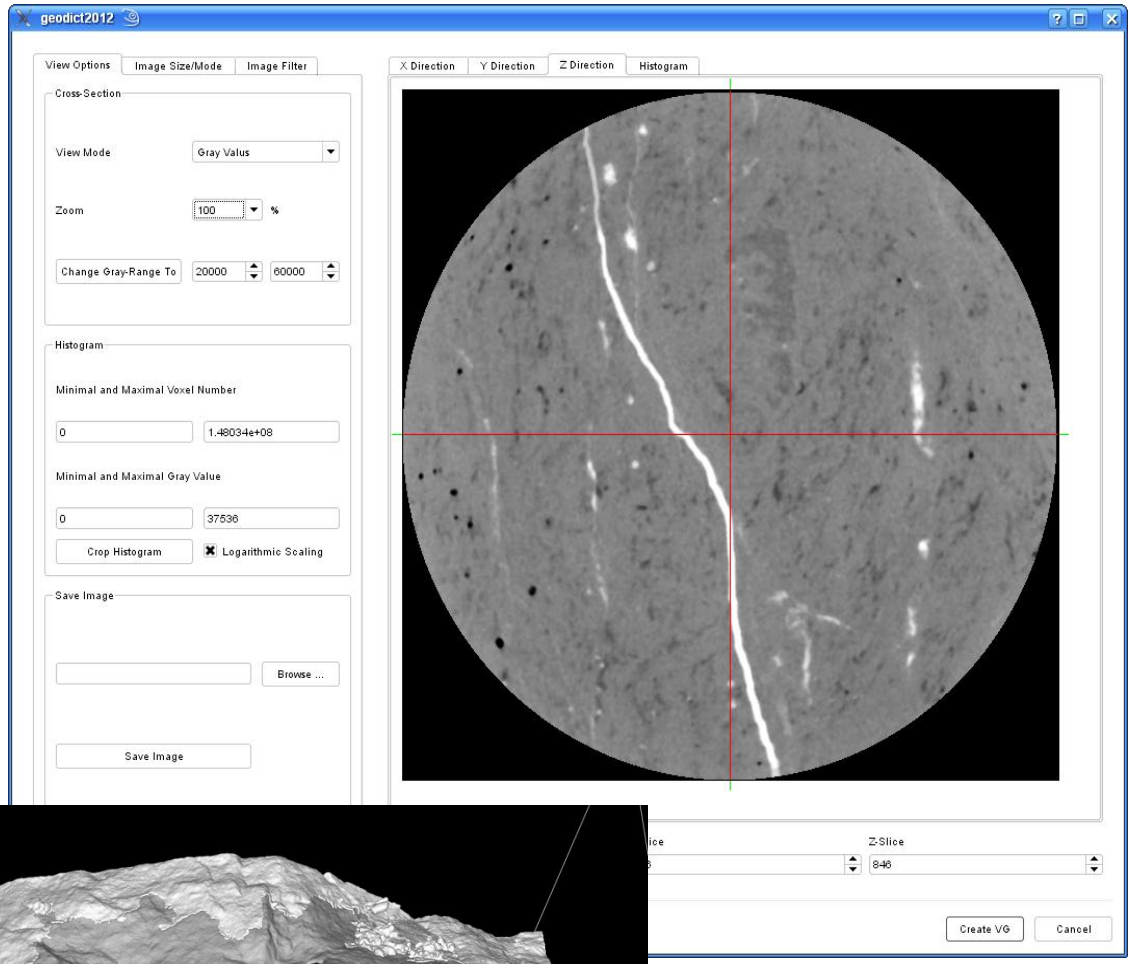
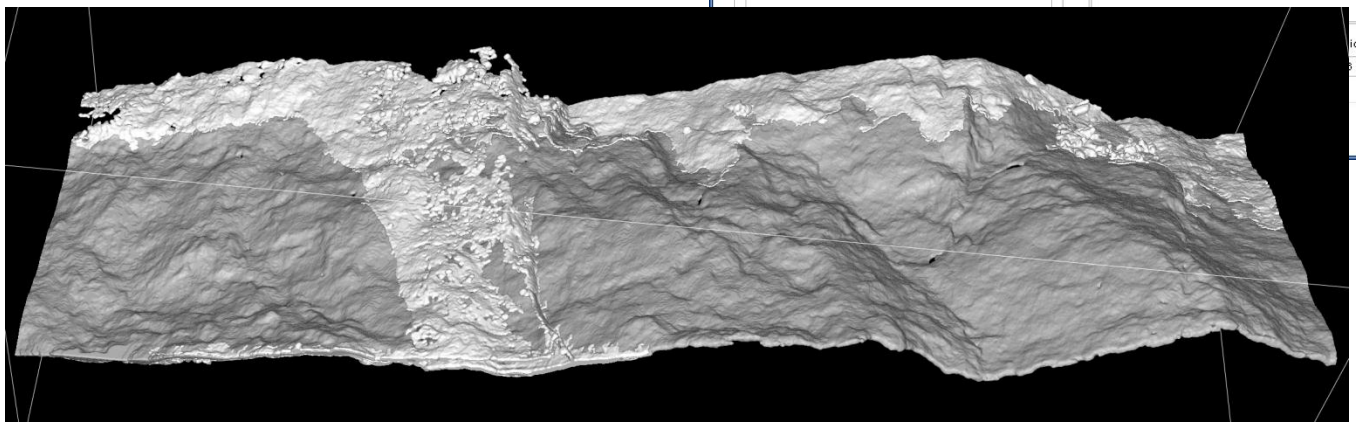
Granite Fracture - CT

- resolution of 80 µm
- segmented: pores, porous material, solid
- size 631x631x1691voxel

(by F. Enzmann et al at the University of Mainz, Institute for Geosciences)





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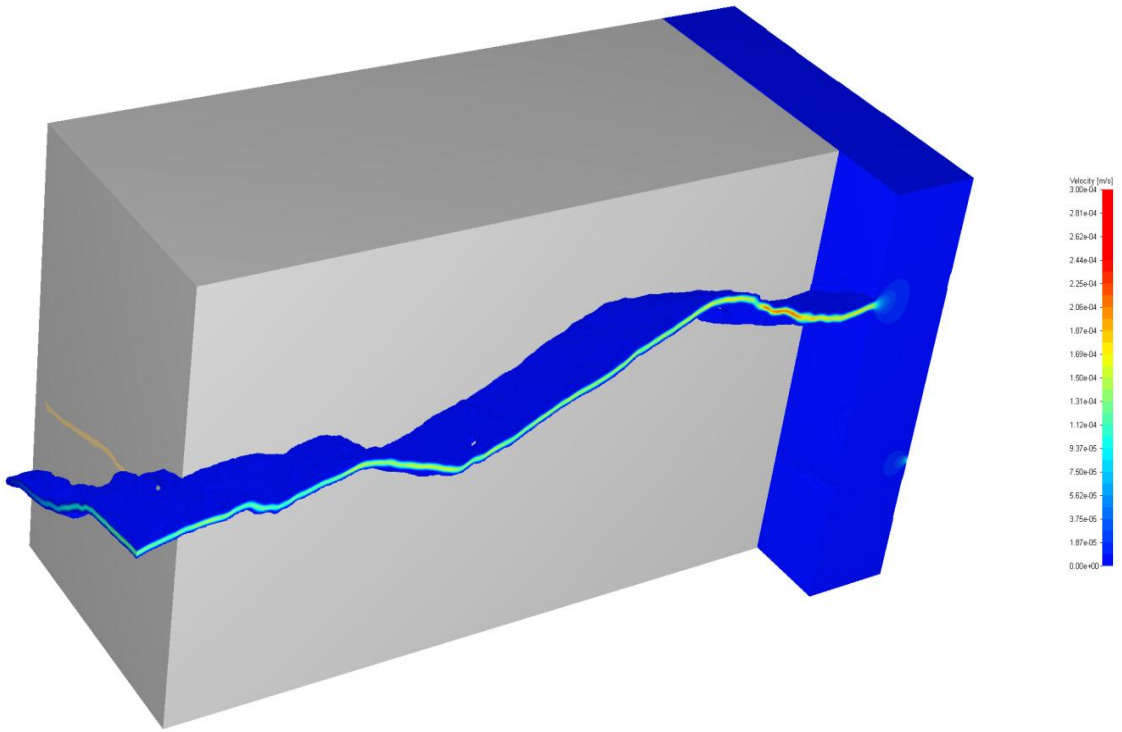
Granite Fracture - The Flow Simulation



incompressible stationary Navier–Stokes equation:

$$-\mu\Delta u + \nabla p + \rho u\Delta u = 0$$
$$-\mu\Delta u + \nabla p = 0$$

- finite volume solver (EFV in GeoDict)
- method is optimized for large voxel grids
- porous material is viewed as solid

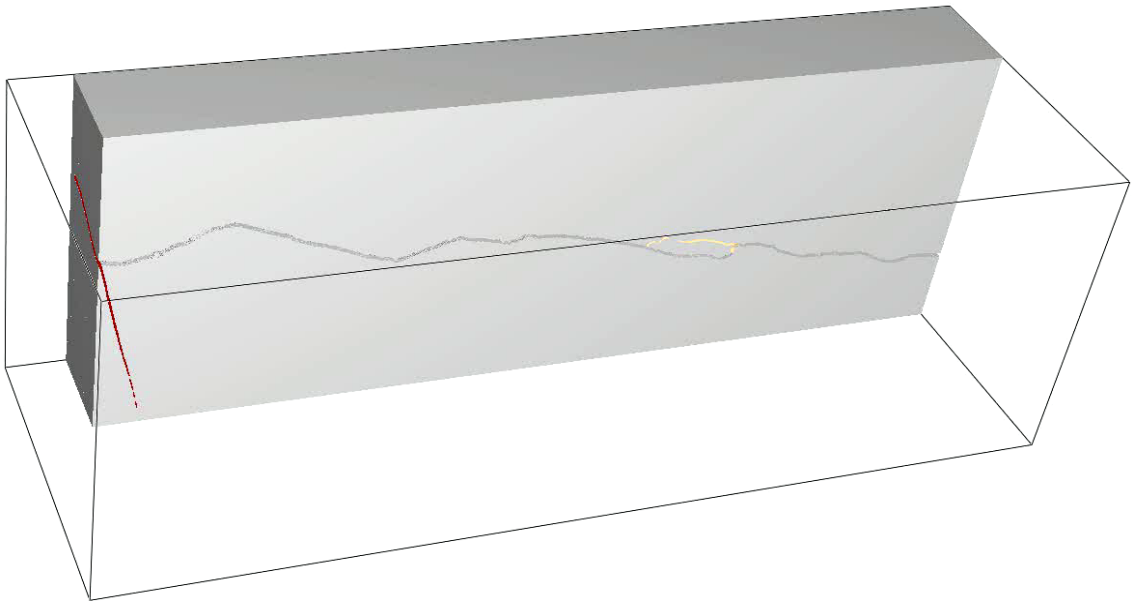
the computational costs for 631 x 631 x 1800 voxels:
8 processes on a 12-core desktop machine, 72 GB RAM, 4 h simulation time

flow simulation was performed for water at 20°C, flow rate 66.8 µL/min

Granite Fracture - The Transport Properties

particle properties:

- diameter 12 nm
- density 4000 kg/m^3
- no chemical processes
- diffusion



=> simulation reflects the impact of fracture geometry on mass transport

interaction model:
particle hitting the fracture walls bounce of, no energy-loss (sieving model GeoDict)

transport simulations => breakthrough curves, particle concentrations

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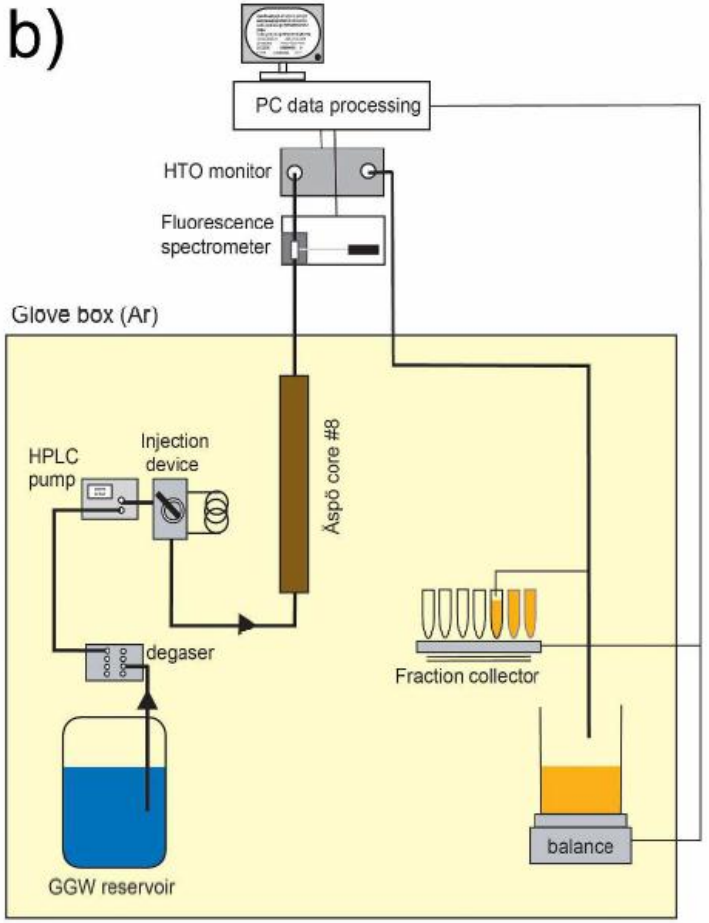
Granite Fracture - Column Migration Experiment

a)

b)



the nanoparticle (quantum dots) transport is experimentally realized by means of column migration experiments at the KIT, Institute for Nuclear Waste Disposal

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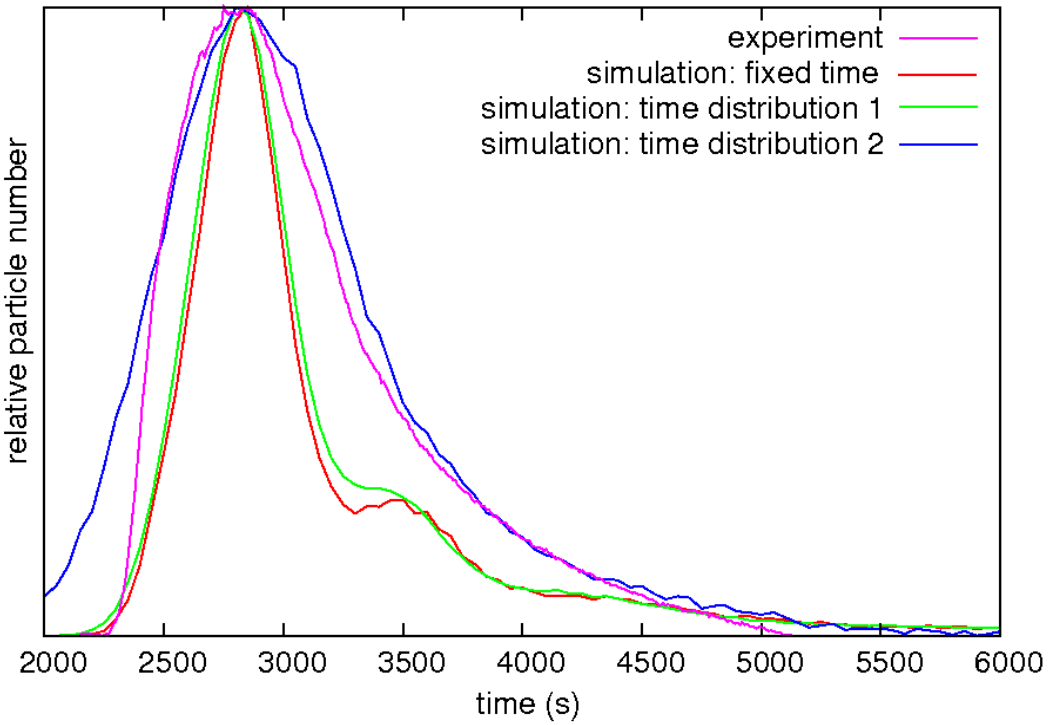
Granite Fracture - Break-Through Curves

simulation:
varying starting times, particle numbers

red: 100,000 particles, fixed time

green: 1,000,000 particles, Gaussian distributed start times, standart deviation 100 sec

blue: 100,000 particles, standart deviation 300 sec



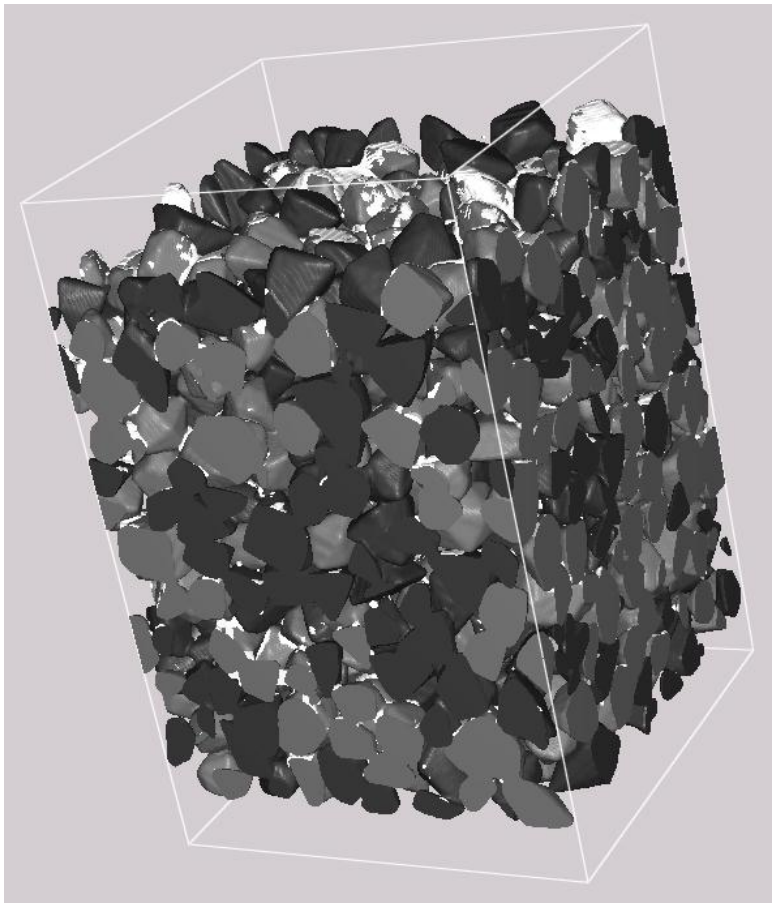
experiment: 66.8 µL/min, exact times and positions of particles entering the fracture unknown

=> changing start times the simulation matches the experimental result very well

Charcoal Water Filter – Virtual Model

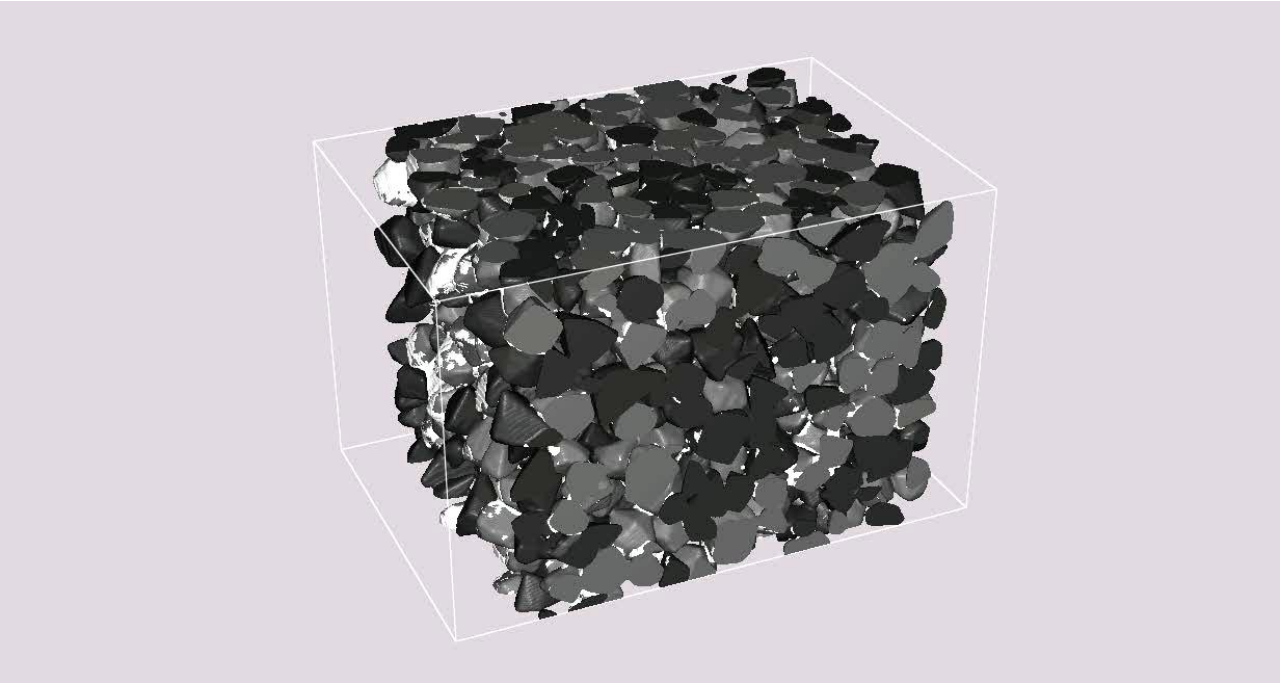
material model based on CT-images of charcoal water filters:

- size and shape distribution of the grains and the (outer) SVF (diameters 100 – 200 micron)
- voxel length 4 micron (200x200x300 Voxel)
- the inner structure of charcoal as permeable grains
- the filtration simulation has to be adjusted to experimental data

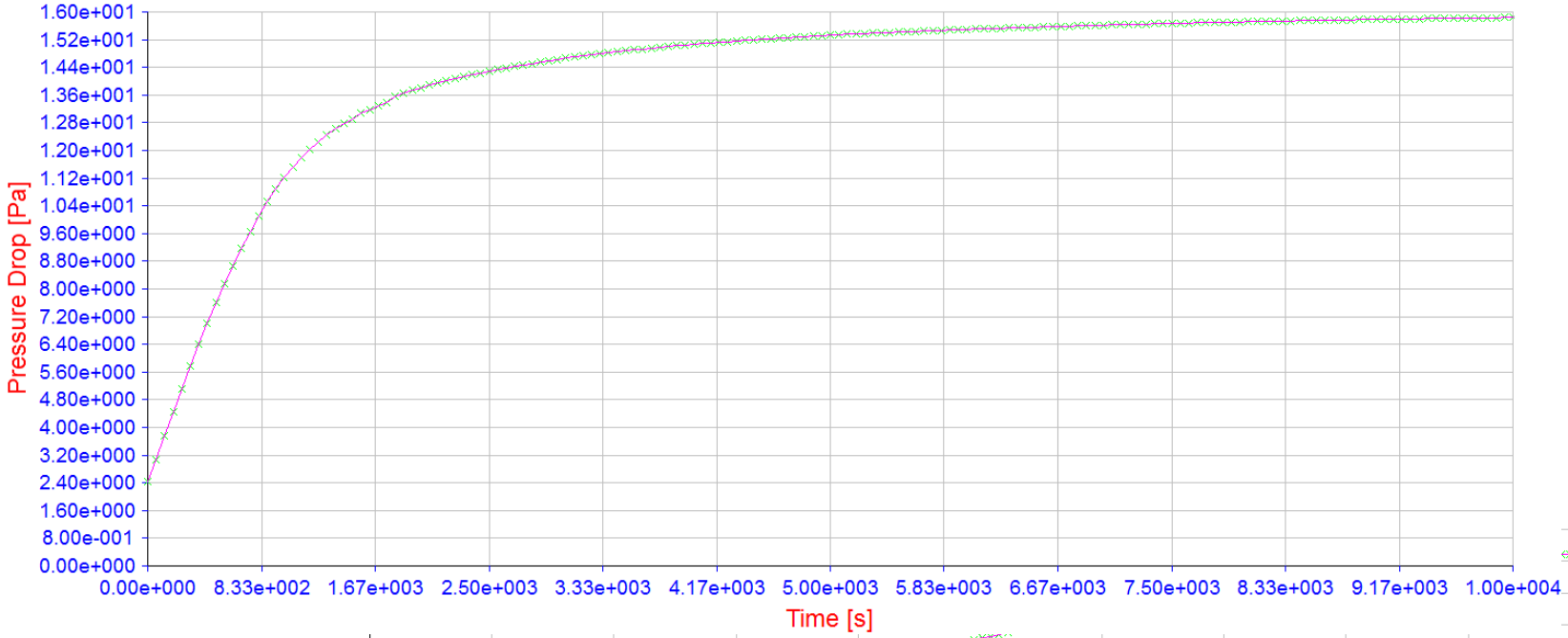


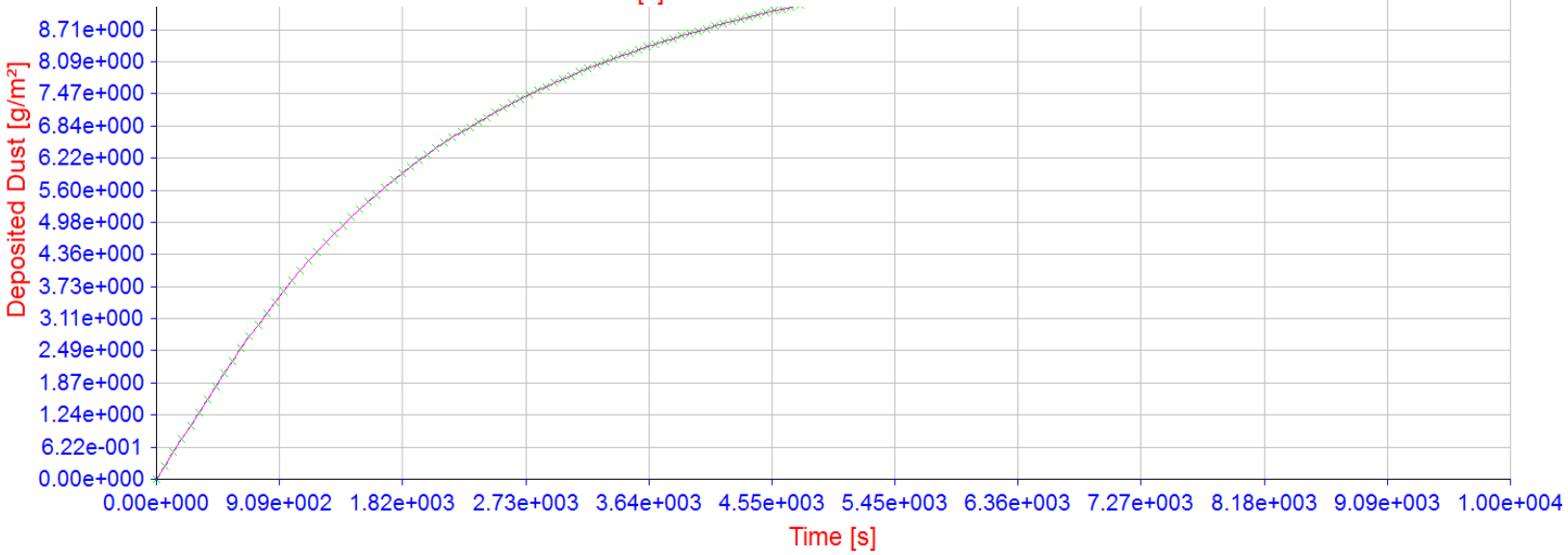
Charcoal Water Filter - The Filtration Simulation

- 150 batches with 200000 particles per batch
- water flow 0.01 m/s
- particle diameter 1 micron



- interaction model between particle and solid: **caught on first touch**
- a voxel on the surface of a grain is filled with ten volume percentages of particles no more particles can enter, the grain surface has reached its adsorption limit
- particles which hit filled surface bounce off with the loss of halve their energy





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Conclusions

3D tomogram of a granite fracture:

- compute flow / transport properties (GeoDict software)
- simulation agree very well with corresponding experimental results

Surface Adsorption

- GeoDict can create models for charcoal filters
- simulation of surface adsorption possible, experimental adjustment needed

Thank You!

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Geometry generator, property predictor and virtual material designer

www.geodict.com

MATH 2 MARKET

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