# PREDICTION OF ADSORPTION AND BREAK THROUGH CURVES BY DIRECT NUMERICAL SIMULATION

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## ABSTRACT

Particle Adsorption, particle absorption and break through curves are of interest in diverse applications like automotive air filters, water filters and subsurface transport settings. They are notoriously difficult to predict because they depend on many parameters such as the adsorption capability of the material and the pore geometry of the porous media. The aim of this work is to propose ways to predict these quantities based on direct numerical simulations with the software GeoDict.

At first an accurate three-dimensional micro-structural representation of the geometry of a porous media is constructed. Examples are the CT image of a fracture in granite, and the computer model of an active carbon filter media based on a micro CT image. Based on the microstructure model the fluid flow through the pores of the media is computed. The flow field is the basis for the third step, the tracking of particles, considering their interaction with the material surfaces and modelling the time-dependent absorption or adsorption on these surfaces.

For the CT image of granite the break through curves were modelled and measured for the same rock sample. On the one hand, tracer particles are monitored, and on the other hand, break through curve simulations were performed on the CT image of the same sample. The comparison shows a good agreement between simulation and measurement.

For the model of the active carbon filter media an iterative filtration simulation, with additional modelling of deposition-dependant surface-adsorption, is performed. The sub-grain porosity of the media is modelled by the effective surface adsorption on the grain surfaces.

## KEYWORDS

Simulation, Absorption Filters, Adsorption Filters, Water Filters, Porous Filter Media

## 1 PARTICLE MIGRATION IN A NATURAL GRANITE FRACTURE

In highly impermeable rock, like granite, fractures represent the only pathways for significant groundwater flow. Such fractures often possess complex geometries, which render complex velocity distributions inside the fractures. Since mass transport of both solute and nanoparticles is strongly coupled to the prevailing flow field, it directly reflects the impact of heterogeneous flow velocity distributions. Mass transport in fractured media is prone to hydrodynamic dispersion and molecular diffusion [1-4] leading to pronounced tailings in breakthrough curves [5]. The lack of detailed knowledge about the fracture geometry often hinders an understanding of laboratory or field results of mass transport. Computer tomography (CT) can be applied to provide detailed spatial information of porous media. CT images were coupled with simulations [6] in the past but most often two-dimensional models were applied [7] and only rarely attempts were made to compare the flow and tracing simulations with experimental data in the same system. In this work the mass transport in a drill core sample of a natural fracture is studied experimentally and numerically. The simulations are done with the GeoDict software [8].

The data set considered in this case study is a micro CT image of a granite fracture. The image was obtained by F. Enzmann at the University of Mainz, Institute for Geosciences. The image has a resolution of 80 µm per voxel.

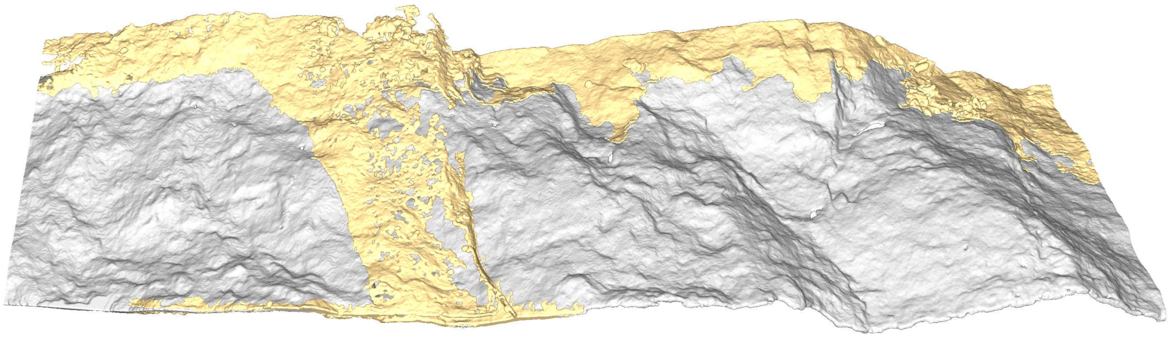

*Figure 1: 3D fracture geometry after segmentation of the tomogram data, porous material (gold), solid / mineral matrix (void), pores (grey).*

The grey-value 3D image is segmented into pores, porous material and solid (mineral matrix). After removing the outer parts of the circular drill core from the image the size of the geometry is 631x631x1691. The resulting segmentation is shown in Figure 1. For the flow and transport simulations an additional inflow region is added, so that the final image has a size of 631x631x1800 voxels.

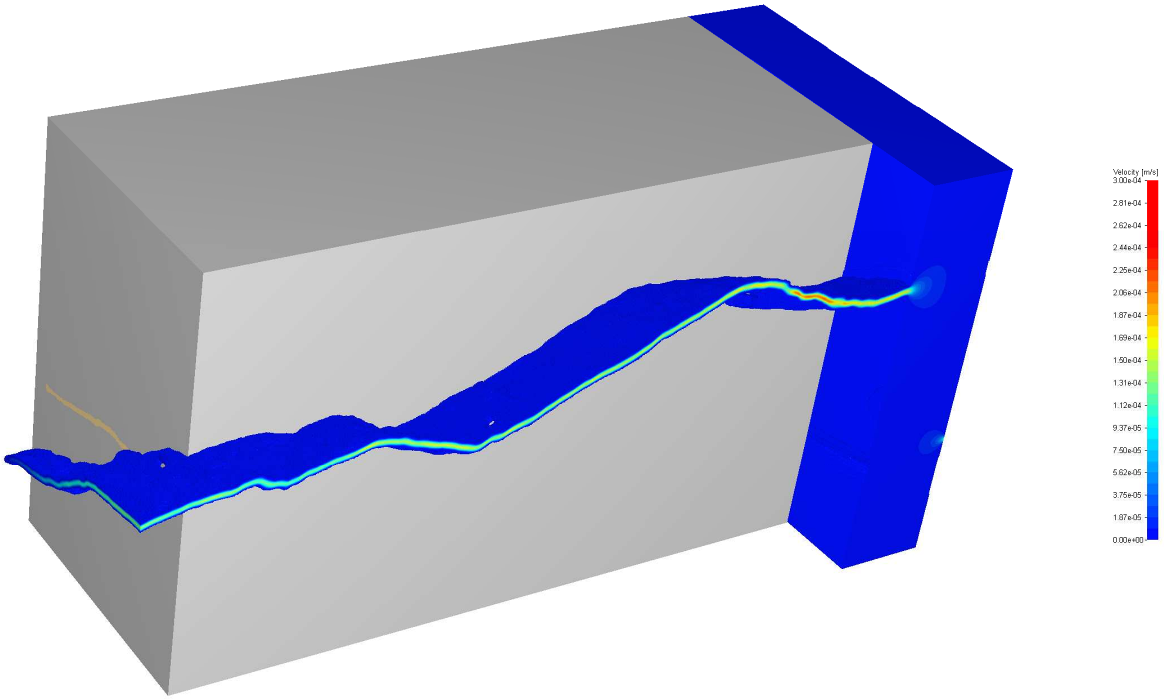

*Figure 1: Velocity of water in the fracture for a flow rate of 66.8 µL/min, solid (grey), porous material (gold).*

We solve the incompressible Navier–Stokes equations using a finite volume solver (EFV in GeoDict [8]), which uses the SIMPLE algorithm [9] and the discretization described in [10]. This method is optimized for large voxel grids, i.e. no re-meshing is necessary. For this flow simulation the porous material is viewed as solid.

The computational costs for 631 x 631 x 1800 grid points are as follows: we used 8 processes on a 12-core desktop machine and needed 72 GB RAM and 4 h simulation time until convergence was archived. The flow simulation was performed for water at 20°C for the flow rate 66.8 µL/min according to a corresponding experiment. A cut-out of the resulting flow field is shown in Figure 2.

The flow-field, calculated is the basis for the computation of the transport properties. The transport-simulation does include diffusion, but does not incorporate chemical processes, thus solely reflecting the impact of the fracture geometry on mass transport.

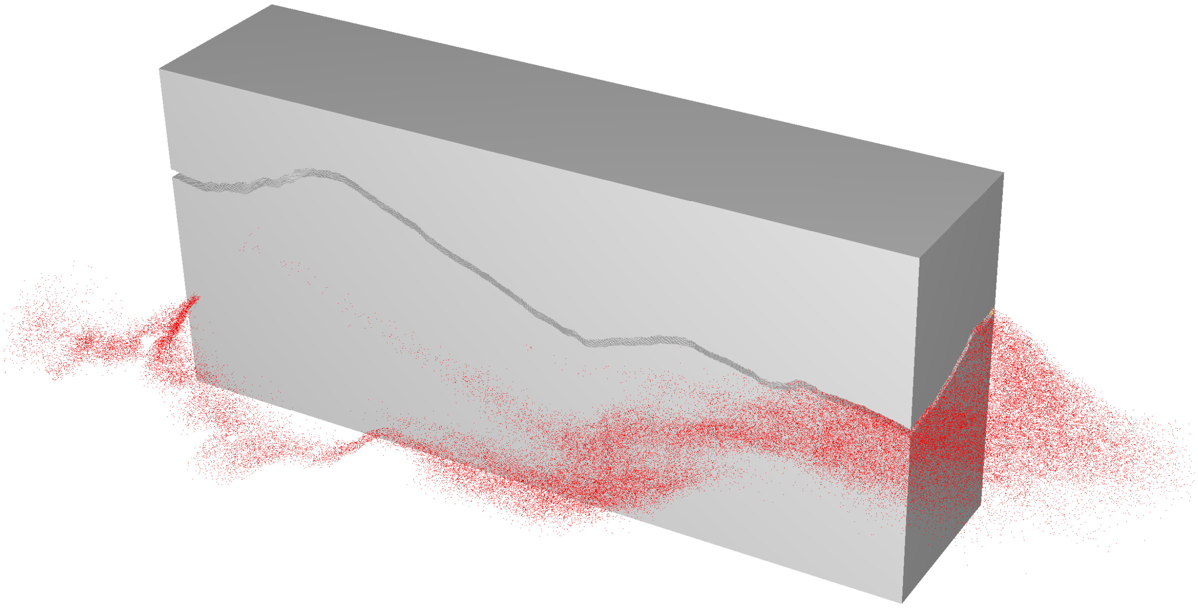

*Figure 3: Visualization of the nano-particles (red) in the fracture for a fixed time, solid (grey).*

For the transport simulation particles with a diameter of 12nm and a density of 4000 kg/m$^3$, where placed in the fracture. These values agree with the experiment, which will be discussed later. The particles are tracked through the geometry, following the complex flow-field (Figure 3).

If a particle hits a fracture wall (solid) it bounces off without the loss of energy (sieving model in GeoDict), where other interaction models are also possible. The transport simulations yield breakthrough curves, characterizing the times at which the particles leave the computational domain through the outflow plane. Breakthrough curves for varying starting times and particle numbers are presented in Figure 4. The red curve shows the result for 100,000 particles, which all started at the same time. For the green curve the starting times of one million particles are Gaussian distributed with a standard deviation of 100 seconds. For the blue curve the standard deviation of the starting times of 100,000 particles is 300 seconds.

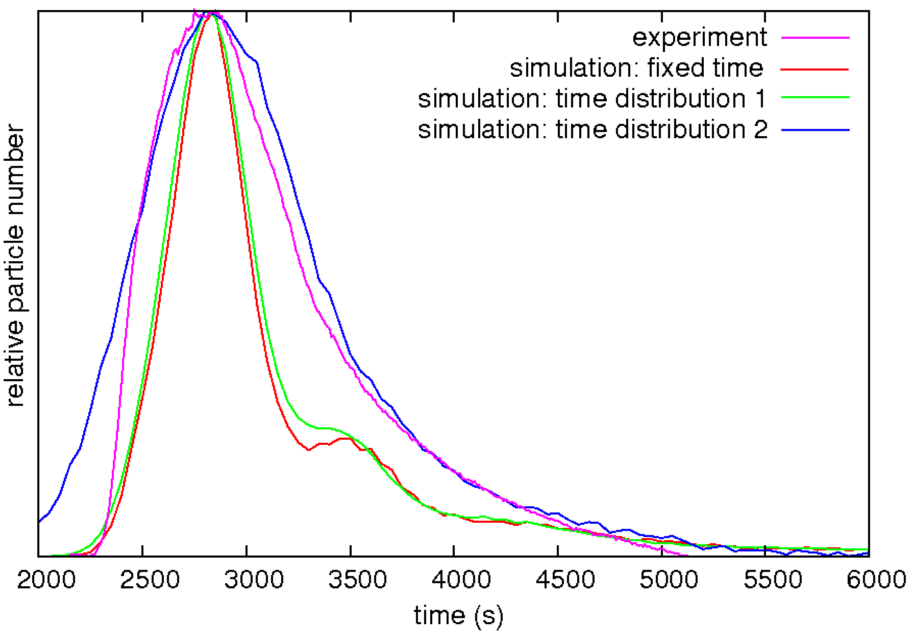

*Figure 4: Comparison of breakthrough curves from experiment and simulation.*

The nanoparticle (quantum dots) transport is experimentally realized by means of column migration experiments at the KIT, Institute for Nuclear Waste Disposal. The general setup of the experiment is explained in [11].

The comparison between the breakthrough curves for the simulations and the experiment is shown in Figure 4. In the experiment the exact times and positions at which the particles enter the fracture are unknown. In the simulation, these quantities are easy to control. Changing the particle start times in a reasonable interval the simulation matches the experimental result very well. Adjusting additionally the particle start positions should result in an even better agreement between simulation and experiment.

## 2 PARTICLE ADSORPTION

GeoDict does not only work on segmented CT images. It has a strong focus on the generation of virtual material models. These models can be used for all kind of property calculations, where examples for filtration properties are shown in [12] and [13]. In this chapter we show filtration property computations with GeoDict using a virtual material model based on CT-images of charcoal water filters.

From the CT-images one can discern parameters like the size and shape distribution of the grains and the (outer) SVF. With this information one can model the geometry of a charcoal filter with the Module SinterGeo of GeoDict (Figure 5). The grain diameter is in the range from 200 to 100 micron and the voxel length of the model is 4 micron. The model does not include the inner structure of real charcoal. To model the effect of the inner structure the properties of the filtration simulation, which I will show in the following, have to be adjusted based on experimental data.

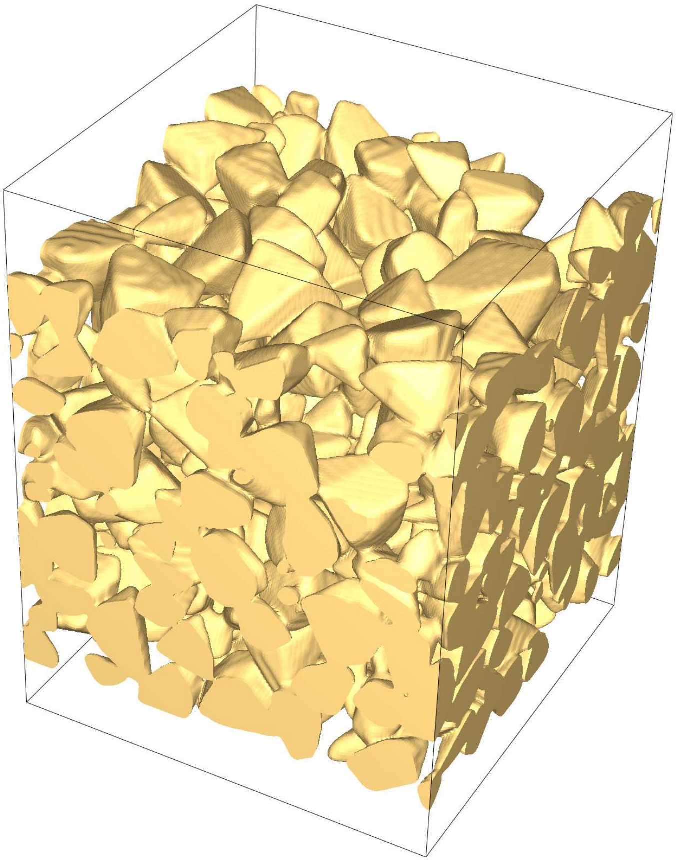

*Figure 5: Virtual charcoal filter media generated with the GeoDict module SinterGeo.*

The filtration simulation with GeoDict is done in an iterative way. At first a flow field is calculated, than a given number of particles is tracked through the geometry. The particles which are caught in the structure change the geometry or the material properties. For that reason a new flow field, followed by a new particle tracking step, is computed. One of these iterations is called “batch” in GeoDict.

For the example we show here 100 batches with 100000 particles per batch are calculated. The water flow velocity is set to 0.01 m/s, the particle diameter is set to one micron and the interaction model between particle and solid is set to "cough on first touch". A particle hitting a grain surface sticks there. If a voxel on the surface of a grain is filled with ten volume percentages of particles no more particles can enter. The local grain surface has reached its absorption or adsorption limit. If further particles hit this part of the grain surface they do not stick anymore, but bounce off with the loss of halve their energy.

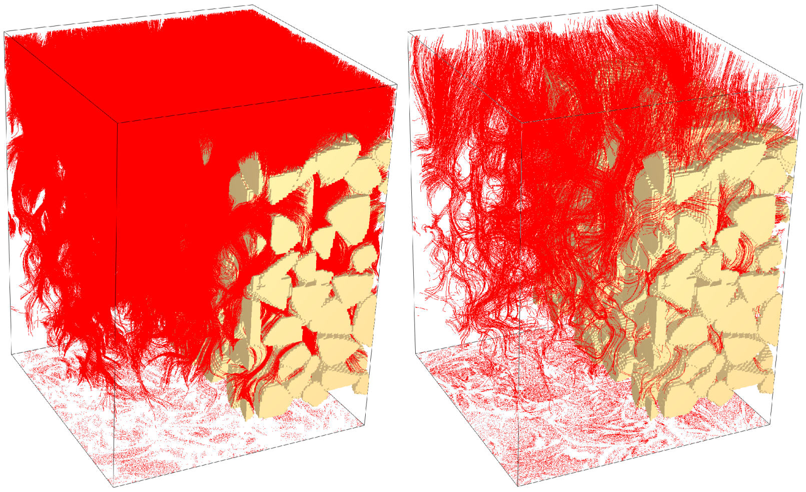

*Figure 6: Filtration simulation with GeoDict, trajectories of filtered particles in red, particles which are not filtered as red pixels at the bottom of bounding box. (Left): batch 1. (Right): batch 100.*

In the beginning of the simulation (during the first batches) nearly all particles are filtered (Figure 6 left) and the filtered particles deposit at the surface of the grains of the media (Figure 7). With increasing time (batch number) less and less particles are filtered (Figure 6 right). The reason for this behaviour can be seen in Figure 7. The surface of the grains, which can be reached by the particles (active surface), gets clogged and the particles cannot be caught by the structure anymore. The absorption or adsorption limit is reached.

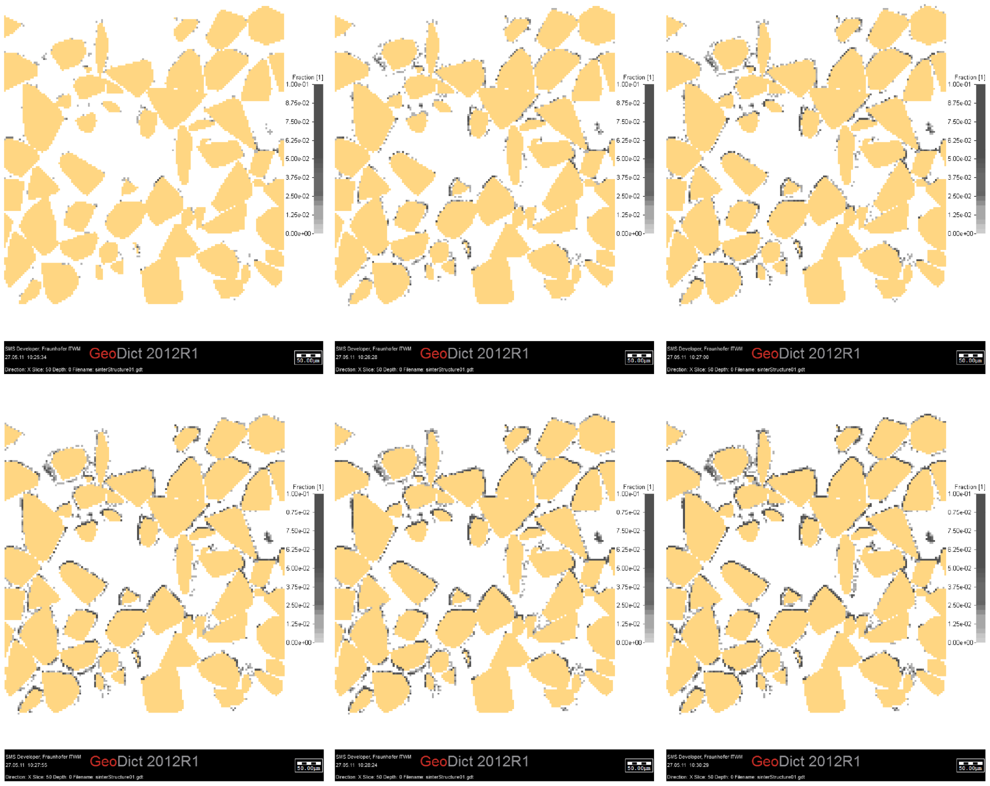

*Figure 7: Filtration simulation with GeoDict, where the geometry is yellow and the concentration of the filtered particles is shown in a gray-scale. From left to right and from bottom to top one sees batch 1, batch 10, batch 20, batch 40, batch 60 and batch 100.*

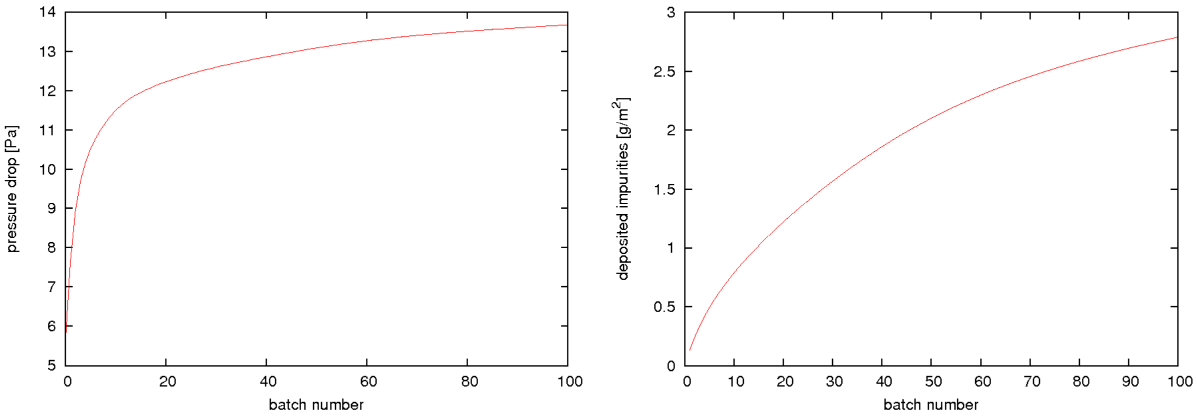

*Figure 8: (Left): Pressure drop in dependency on the batch number. (Right): Deposited impurities in dependency on the batch number.*

The time dependent pressure drop of the filter media is shown in Figure 8. At first, most of the particles get adsorbed by the grains, the pressure drop increases rapidly. Later on, because less and less particles are caught, the pressure drop approaches a constant value. In Figure 8 one also sees the impurities deposited in the media. With time the slope of the graph decreases, as does the filter efficiency. As the filter cannot hold any more particles the graph also approaches a constant value, the maximal amount of impurities the filter can hold is reached.

## 3 CONCLUSIONS

In the first chapter the flow and transport properties of a segmentation of a CT-image were studied. Similar simulations of flow and tracer particle transport are possible with GeoDict for all kinds of natural or manufactured porous materials, revealing the complex influence of the material geometry on the flow, transport and filtration properties.

In the second chapter a way to model the filtration properties of a charcoal water-filter media with GeoDict was demonstrated using a virtual geometry model. The simulation helps to understand filtration processes and predicts filtration properties.

GeoDict is a powerful tool to model, analyze, visualize and predict filtration properties of porous media. The easy to use software is optimized to work fast on large voxel meshes. Furthermore GeoDict can compute e.g. the permeability, elastic properties, pore size distribution, diffusivity, thermal and electrical conductivity of a porous media.

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