Status update of the modelling work

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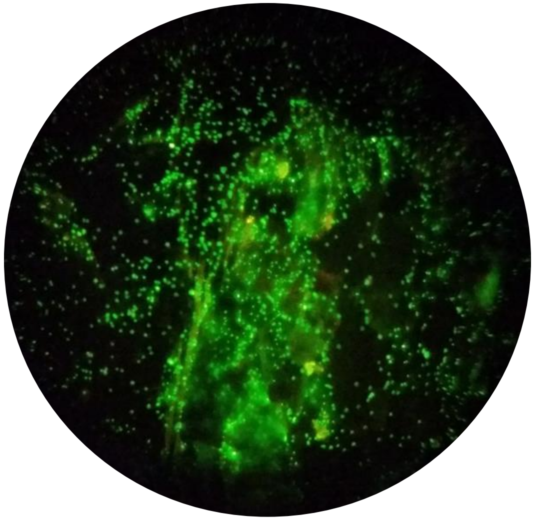
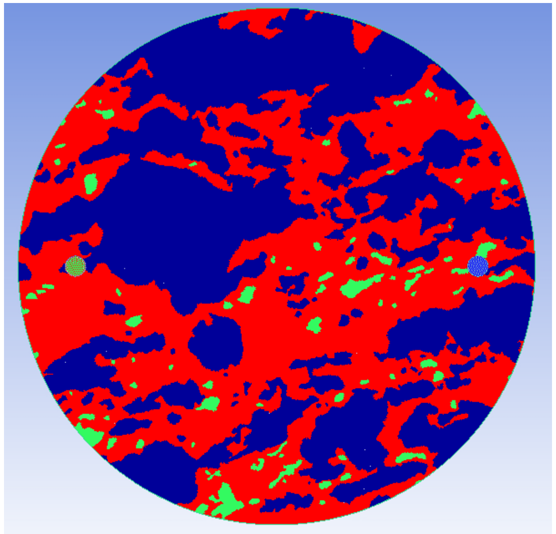
Institute for Nuclear Waste Disposal (INE)





Activities within CP BELBaR

Karlsruhe Institute of Technology

Focus: Impact of fracture geometry on bentonite erosion and colloidal transport

a) Use of 3D natural fracture flow field data and natural fracture aperture data to calculate bentonite erosion rates using the approach presented by Moreno et al. (2010)* (see Deliverable 5.2)

b) Modelling of bentonite erosion in natural fractures: Couple INE fracture model to KTHs and/or VTTs „simplified " erosion model

c) Colloid /particle transport in synthetic fractures (modeling of flow cell experiments)

*SKB, 2010. Modelling of erosion of bentonite gel by gel/sol flow. TR-10-64 Svensk Kärnbränslehantering AB, Stockholm, Sweden.

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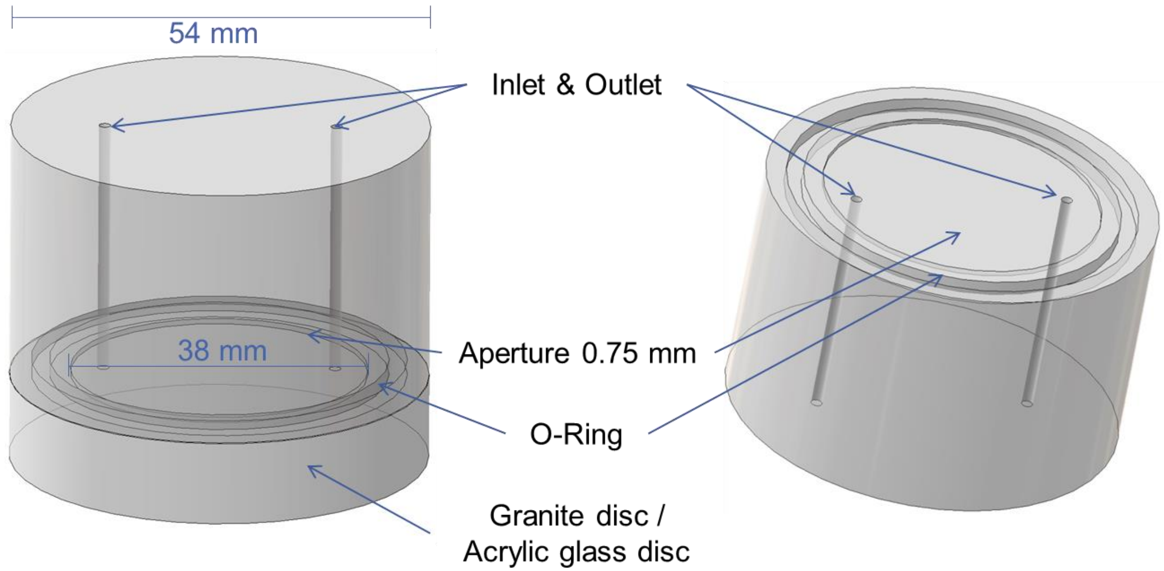
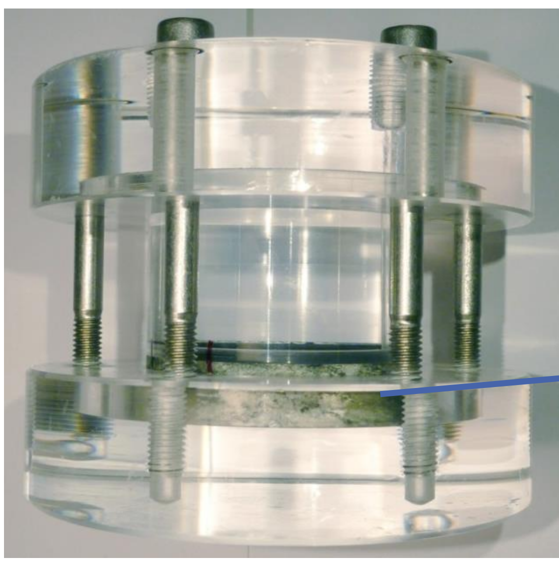
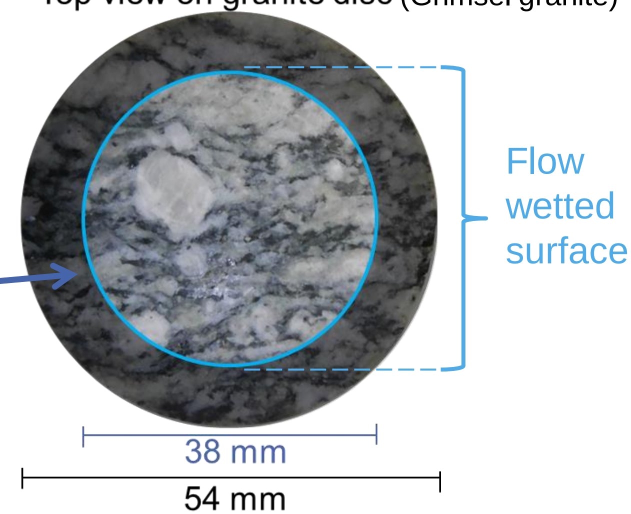
Colloid transport in synthetic fractures

Artificial fracture flow cell

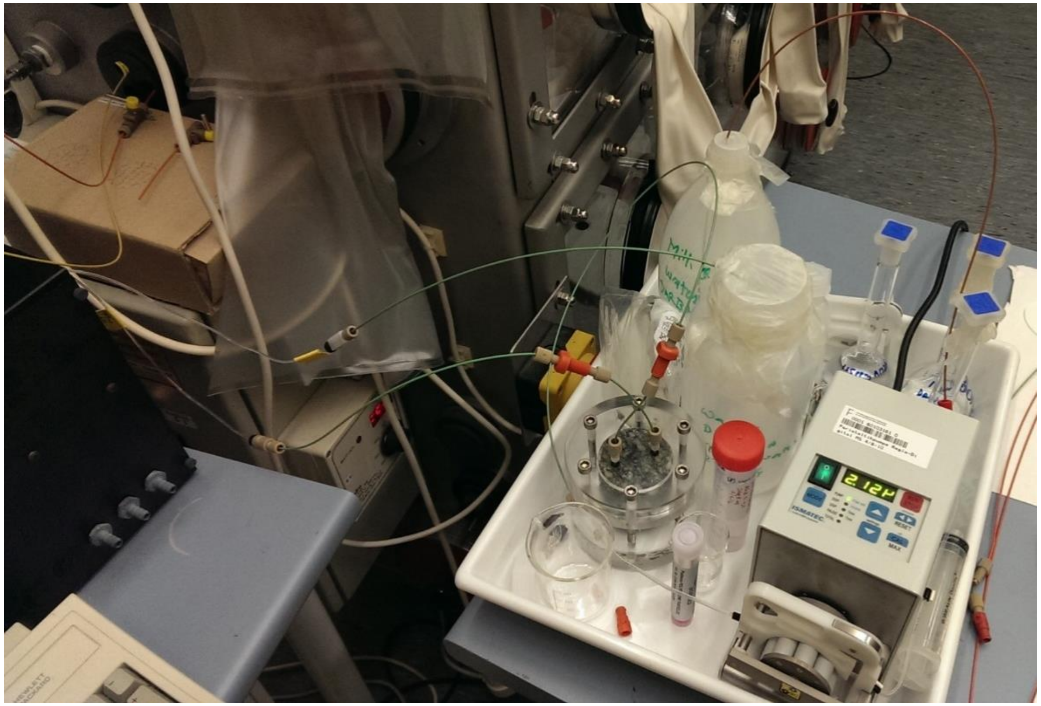


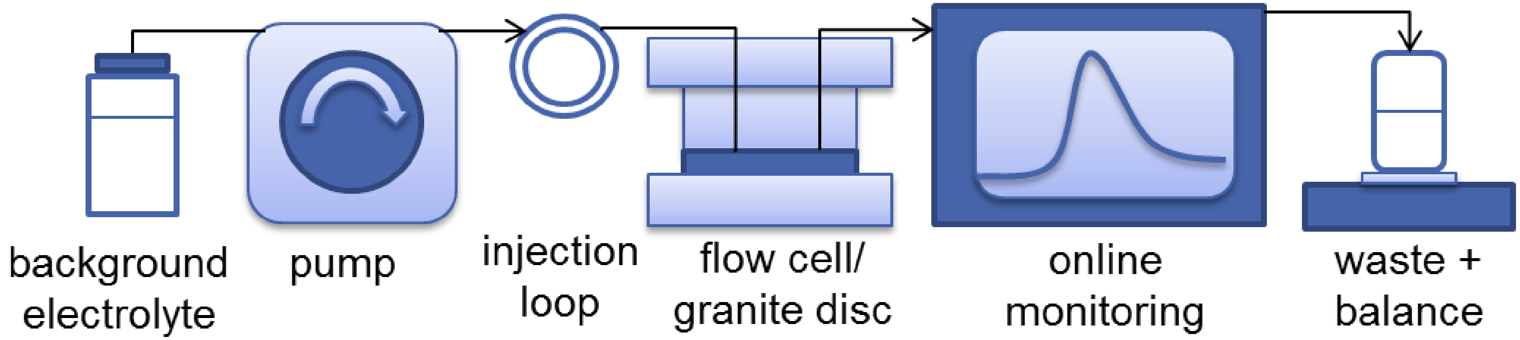


Top view on granite disc (Grimsel granite)



Colloid transport in synthetic fractures

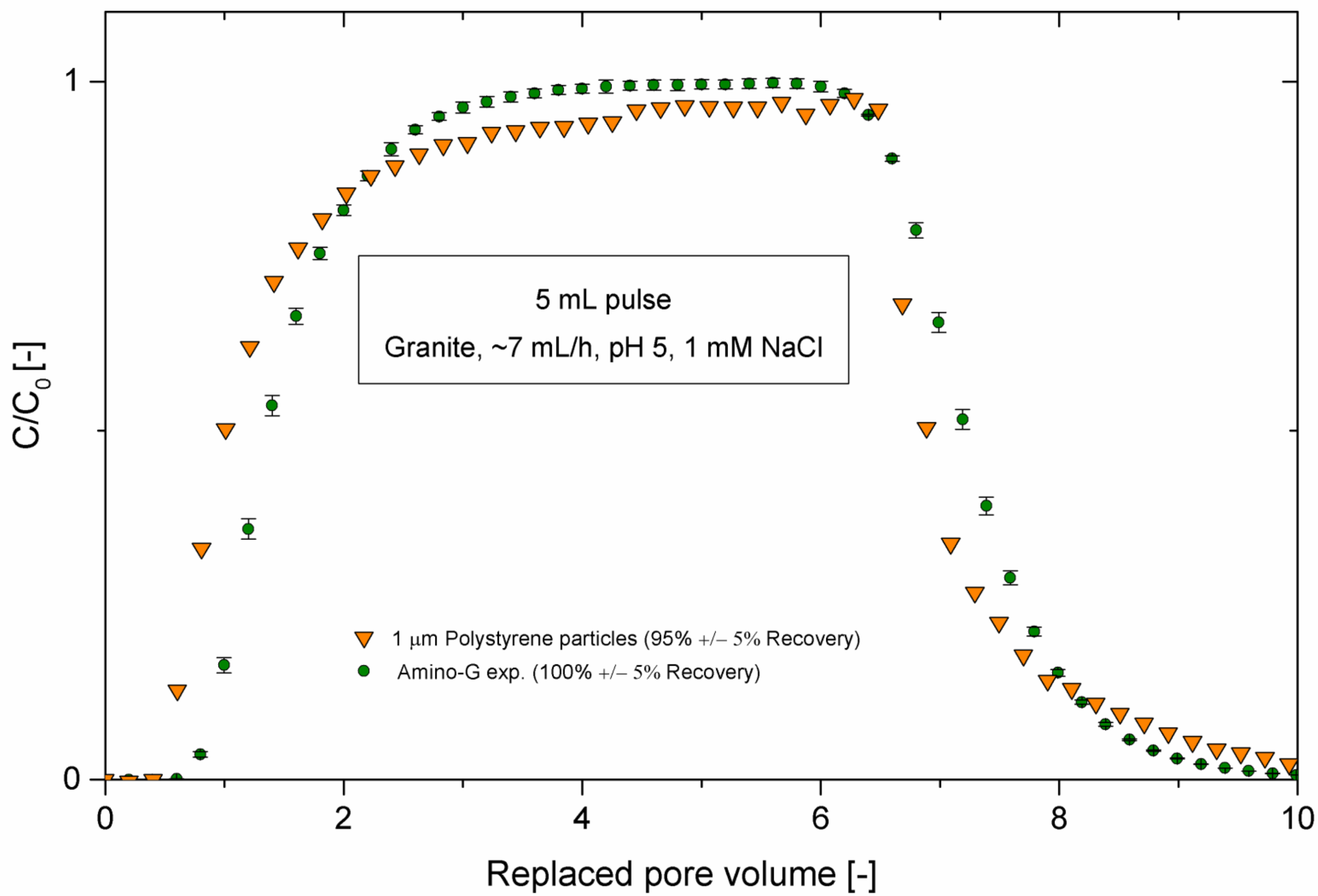




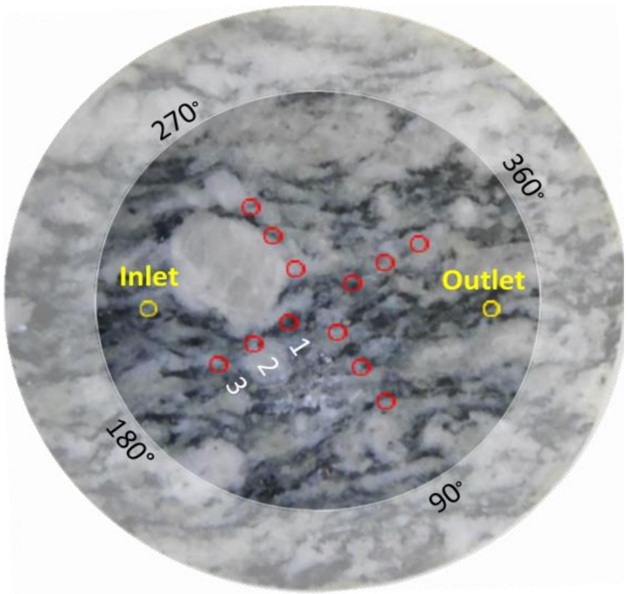
Experimental parameters

Fracture surface type	Granite or acrylic glass
Open fracture width	0.75 (0.4–1 mm)
Colloid size/material	25 & 1000 nm polystyrene particles (+ natural bentonite colloids)
pH	5 and 9.6
Flow conditions	laminar flow conditions (2–172 mL/h ≙ Re 0.015–1.34)
Ionic strength	0.001–1.7 M NaCl
Temperature	20 °C (room temperature)

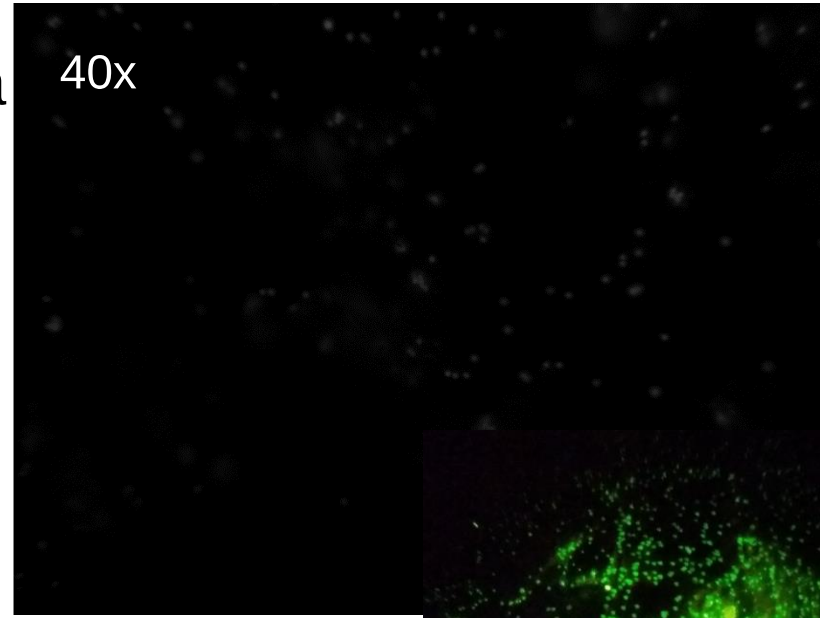
Colloid transport in synthetic fractures



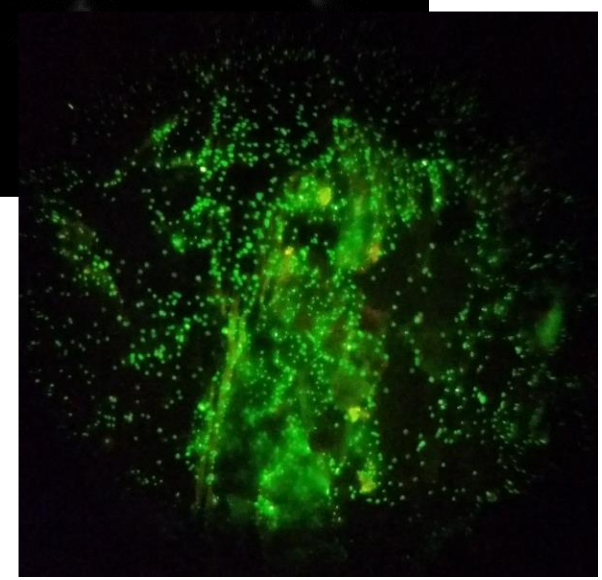
Post-mortem analysis using fluorescence microscopy to visualize 1 µm particles



Camera mode

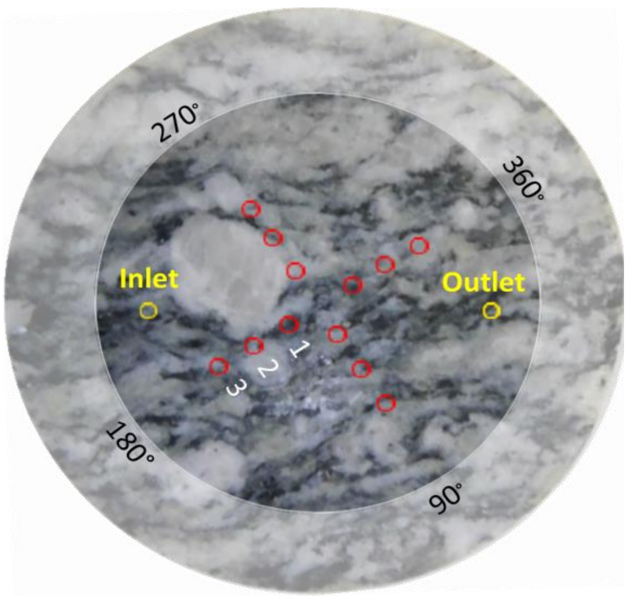


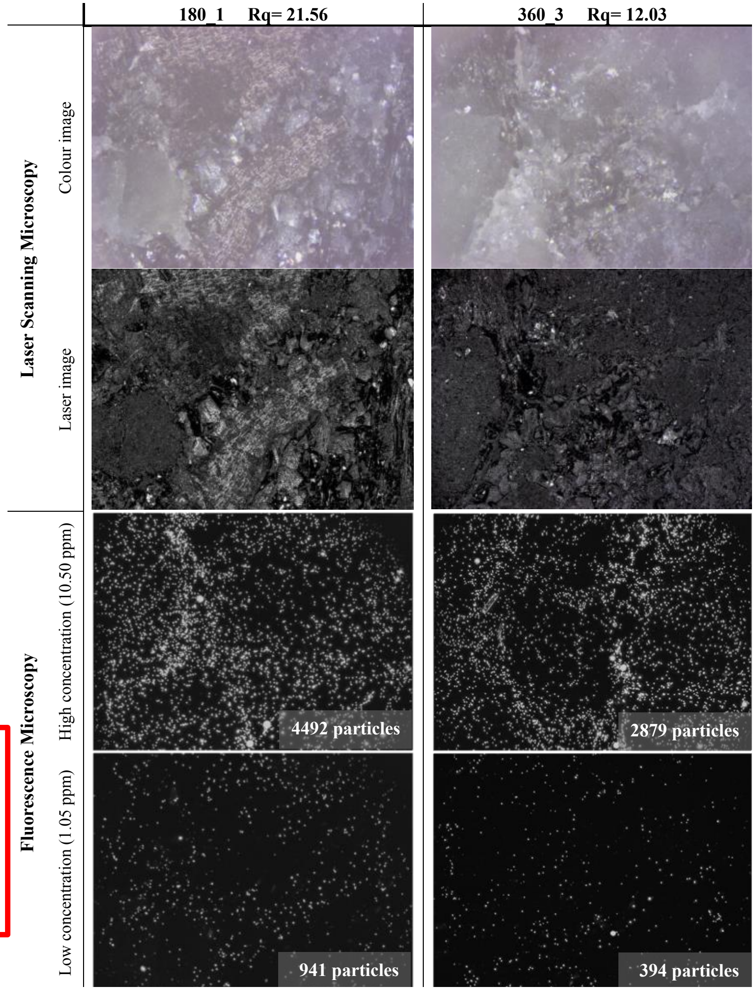
View through the ocular



Colloid transport in synthetic fractures

Post-mortem analysis using fluorescence microscopy to visualize 1 µm particles



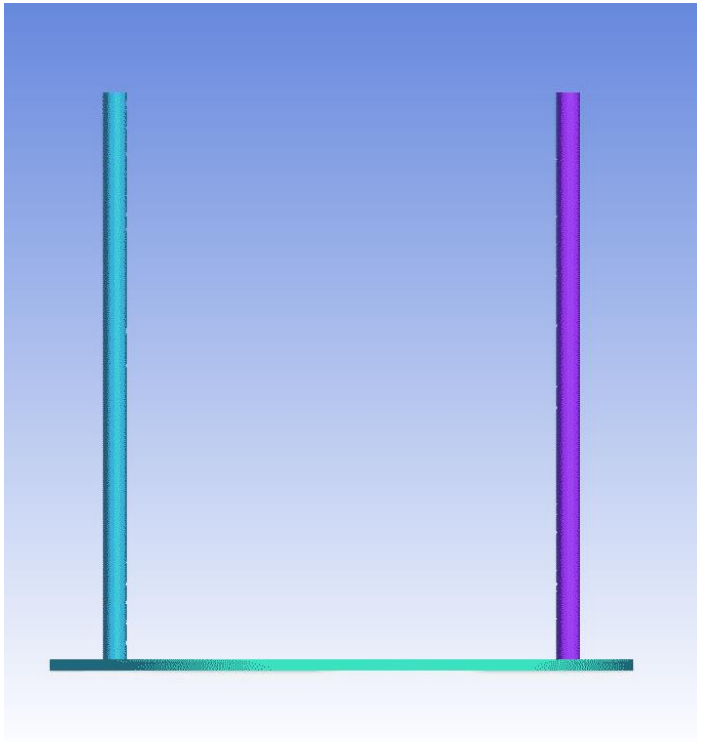


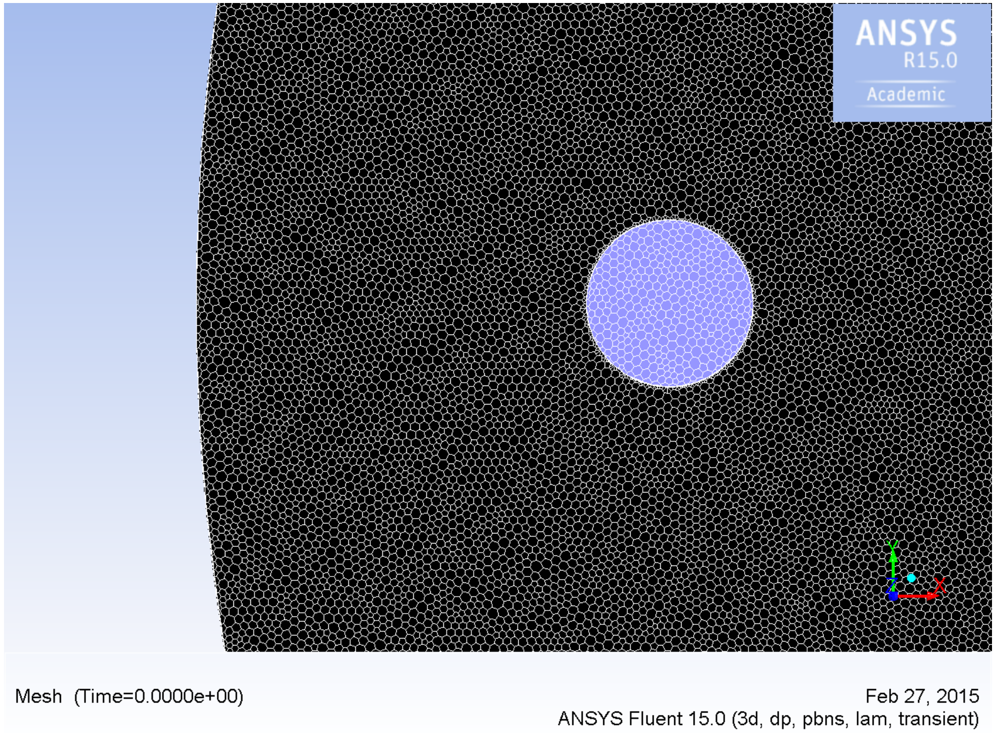
Concentration (ppm)	Retention [%] Breakthrough curve	Retention [%] fluorescence microscopy
10.50	3.80	0.16
1.05	3.99	0.34

Model parameters

Element type	Polyhedra or tetrahedral with boundary layers (~1-3 Mio.)
Flow	Stationary incompressible Navier-Stokes
Particles	Lagrangian tracking 1000nm polysterene colloids (1045 kg/m^3) Monodisperse (polydisperse possible) Spherical (shape correction possible) No charge Pulse or step injection 10k - 1 Mio. particles (~1-0.001 % of experiment) One-way coupling to flow
Forces	Drag, gravity, (Brownian motion), (electrostatics),…
Particle-Wall conditions	For “minerals” => attachment probabilities from AFM (pH dep.) All other walls => bounce/reflect

Colloid transport in synthetic fractures

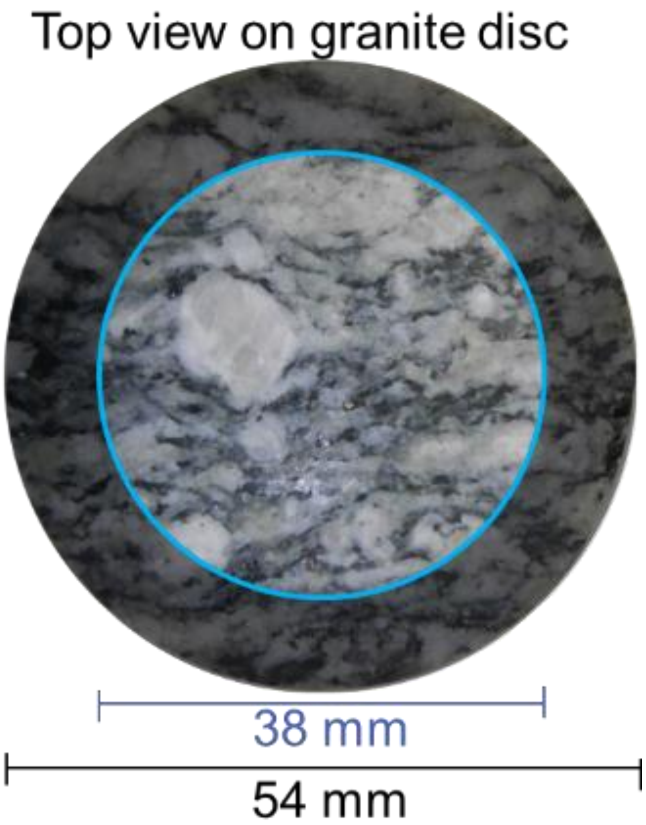


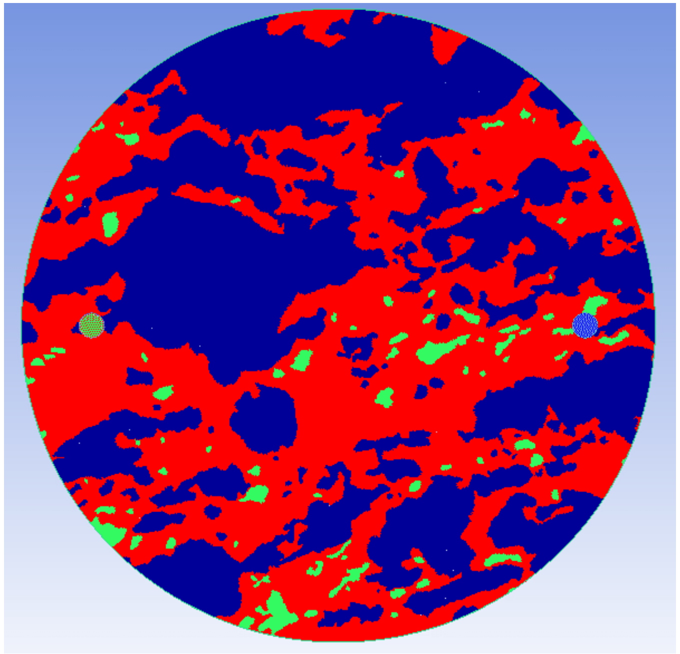


- E.g. polyhedral mesh consiting of ~3.5 million elements
- Test with different mesh types (tetras with BL, etc..)

=> „Mesh refinement study“

Colloid transport in synthetic fractures





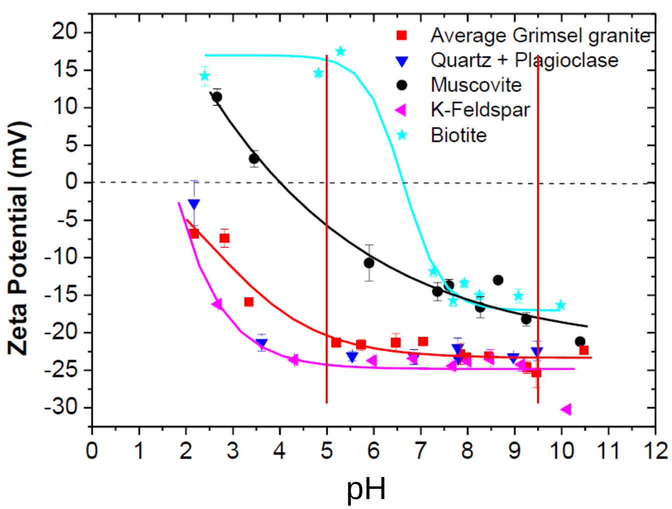
Colloid transport in synthetic fractures

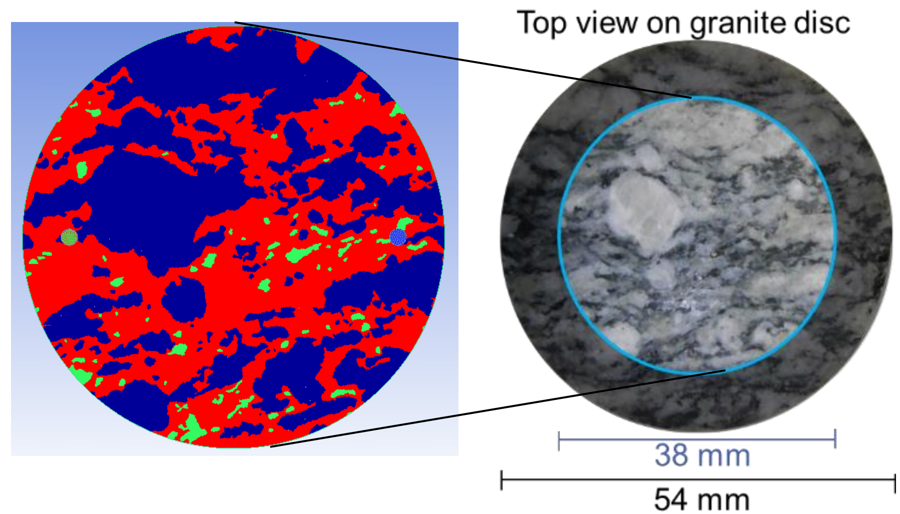
Table 1 Mineralogical composition of the Grimsel granodiorite samples used in this study

Mineral	Sample 1 (vol%)	Sample 2 (vol%)
Plagioclase	39.0	34.0
Quartz	28.4	37.2
Potassium feldspar	21.6	12.8
Biotite	5.0	7.8
Muscovite + sericite	2.6	1.6
Epidote	1.2	1.0
Amphibole	1.8	4.6
Chlorite	0.2	0.4
Carbonate		
Titanite	+	0.6
Apatite		
Opaque minerals	0.2	+

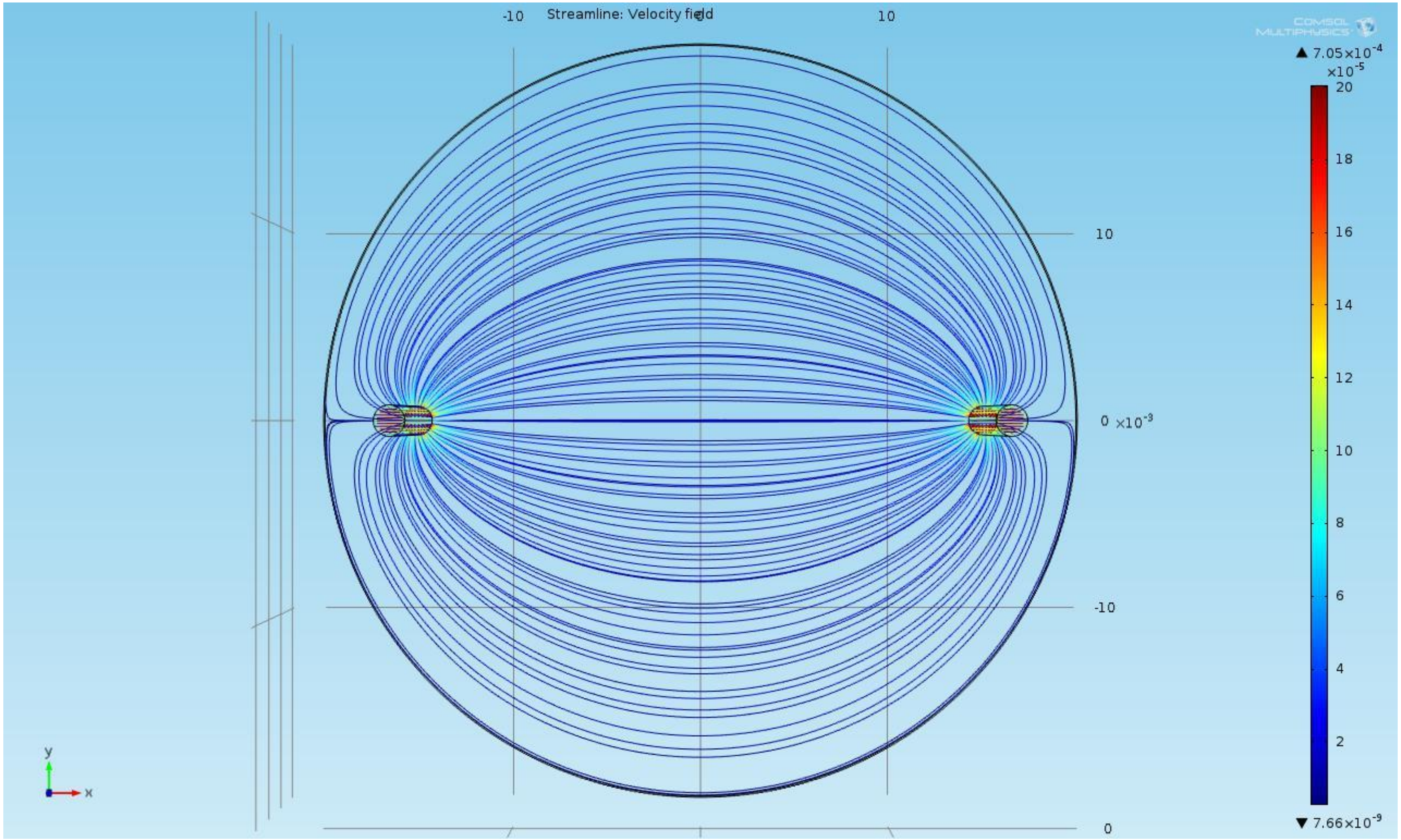
Jokelainen et al. 2013 JRNC

Mineral phase	Full disc (%)	Flow wetted disc (%)
Feldspar + Plagioclase	43.1	48.2
Quartz	46.9	49.2
„Biotite“	10	2.6





Colloid transport in synthetic fractures



Colloid transport in synthetic fractures

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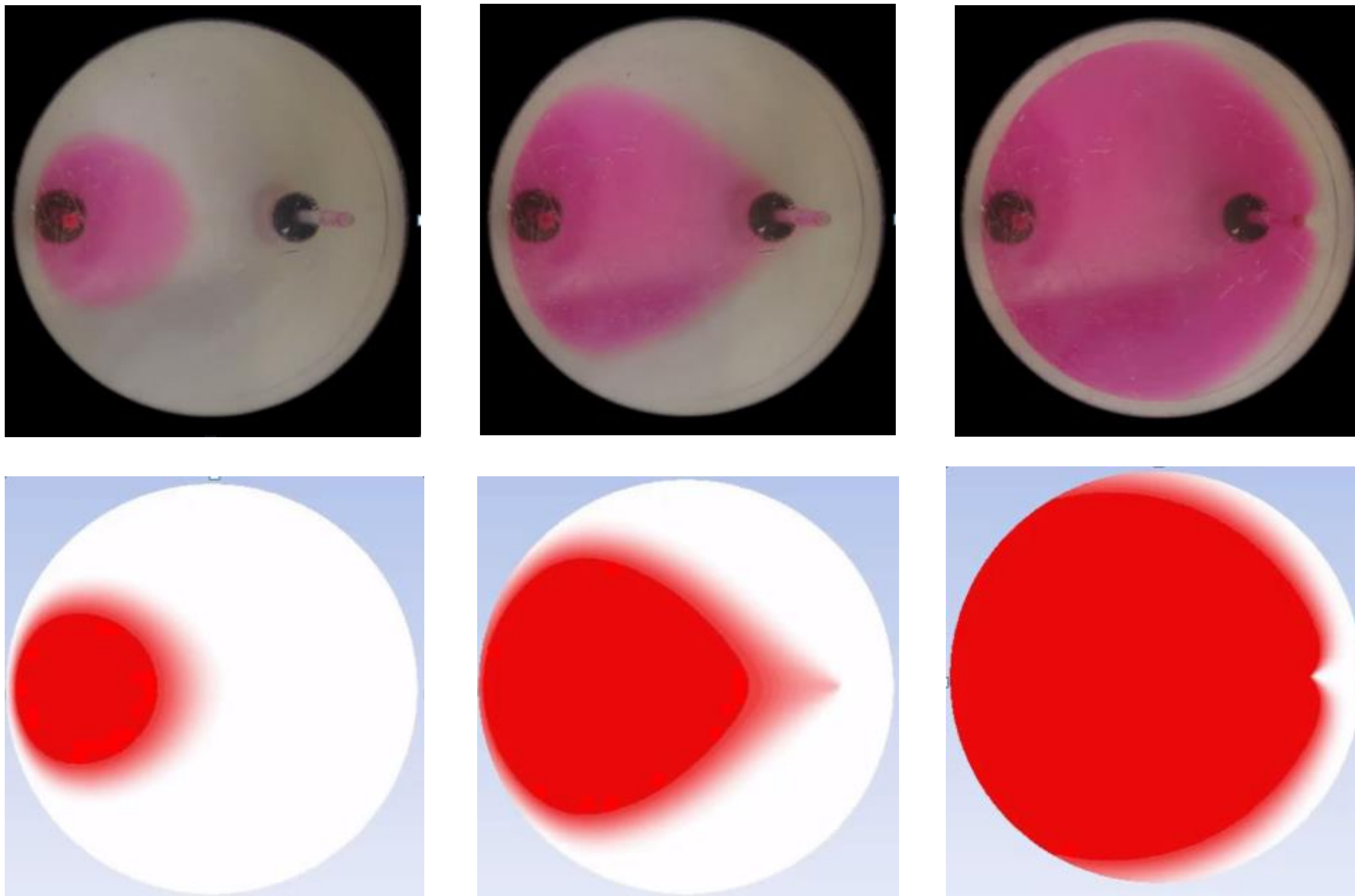
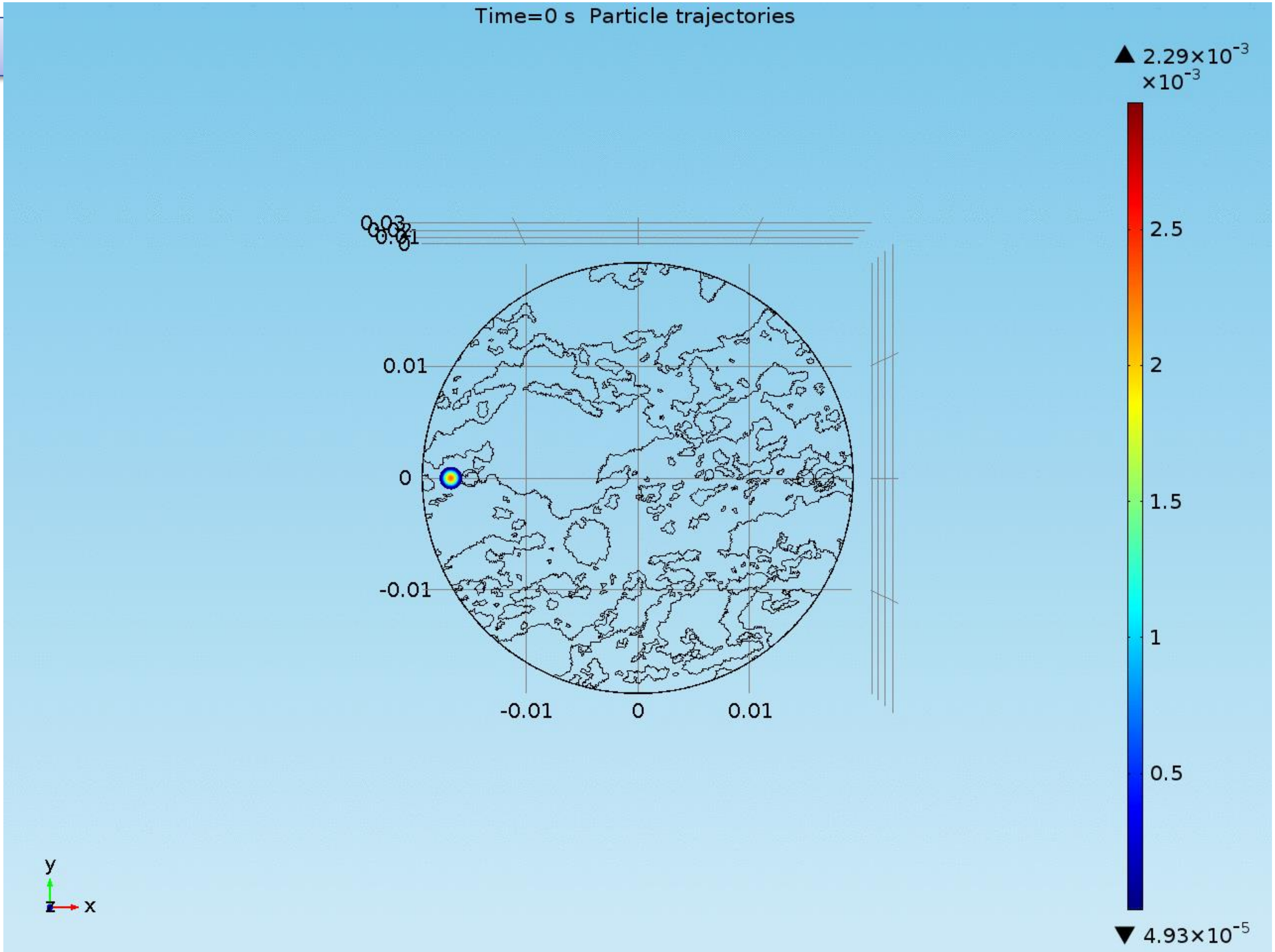
Solute tracer (Rhodamin-B)

Experiment

Model





Time=0 s Particle trajectories
2.29×10-3
×10-3
2.5
2
1.5
1
0.5
4.93×10-5
0.01
0
-0.01
-0.01
0
0.01
y
x

Colloid transport in synthetic fractures

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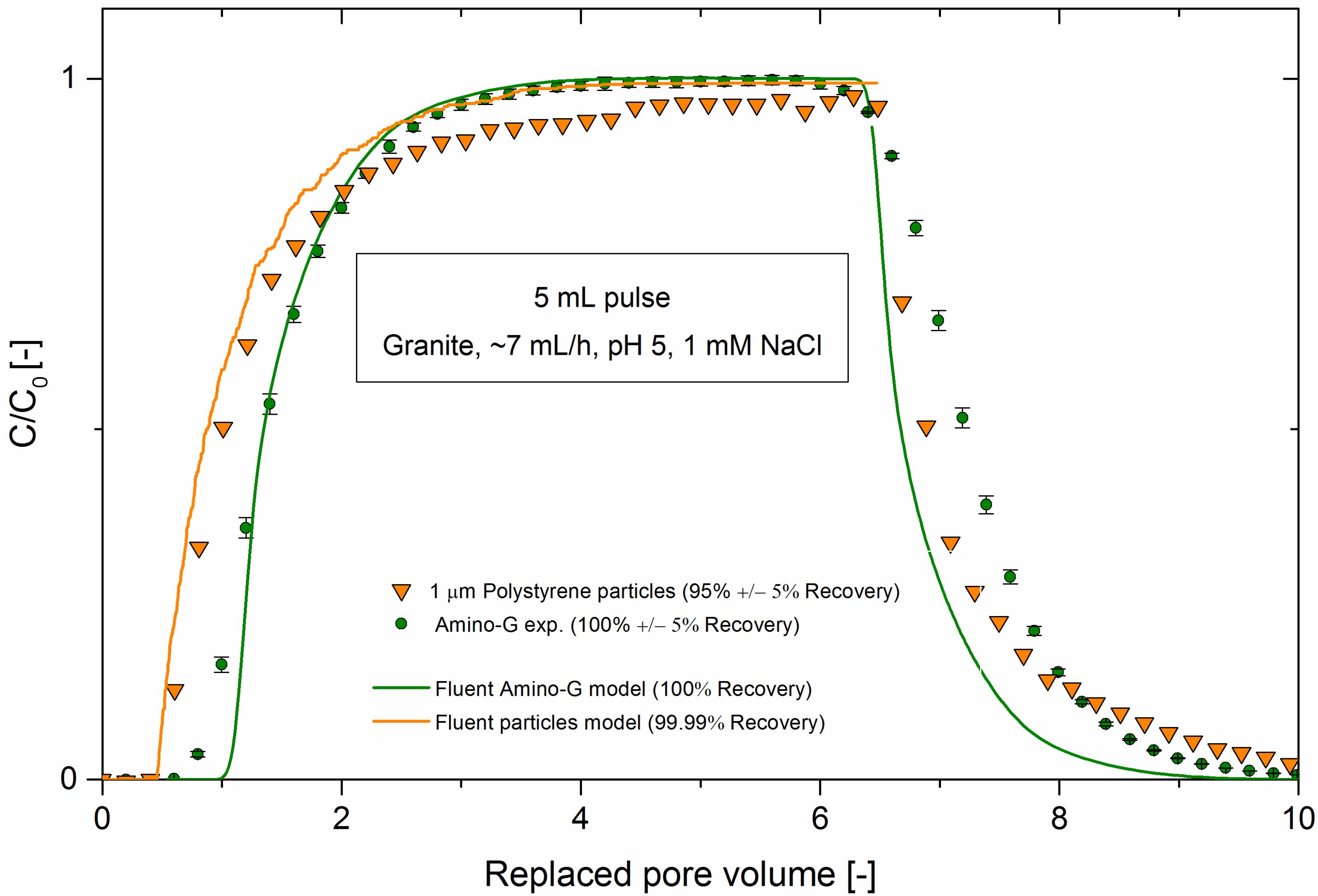

Colloid transport in synthetic fractures

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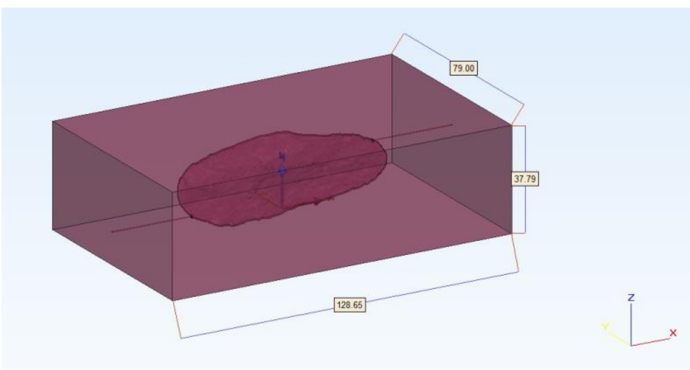
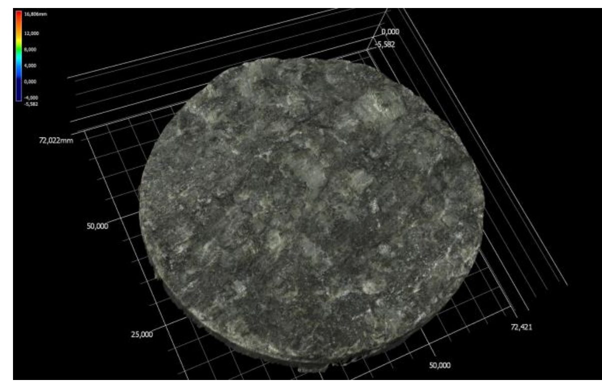
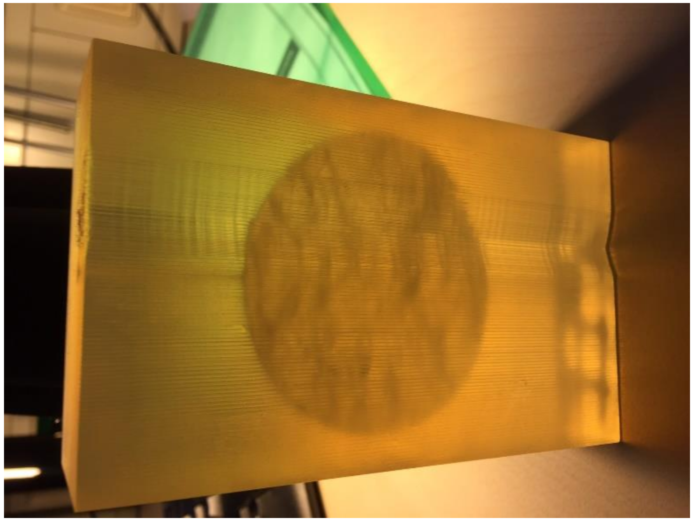
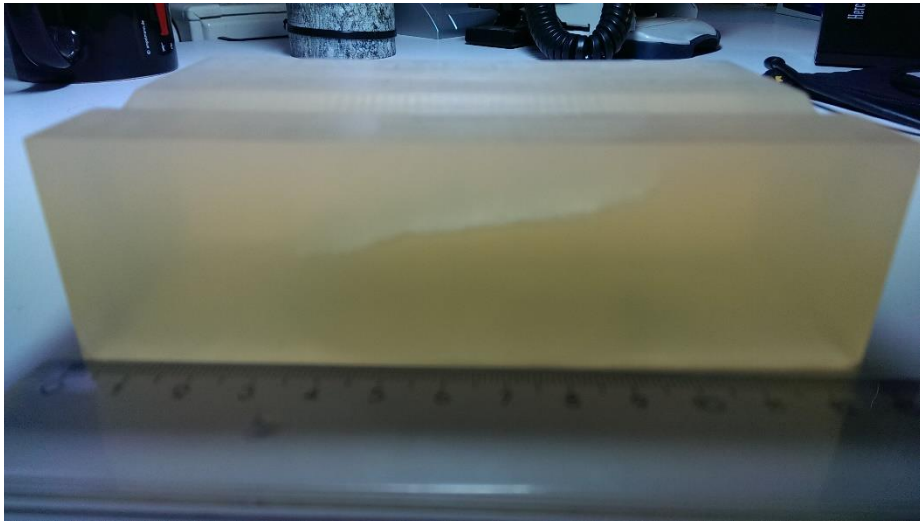




- Grimsel matrix core artificially cracked to obtain fracture surfaces
- Fracture surfaces scanned with a Laser-scanning microscopy (~few µm resolution) => digital data used for model construction

Colloid transport in synthetic fractures





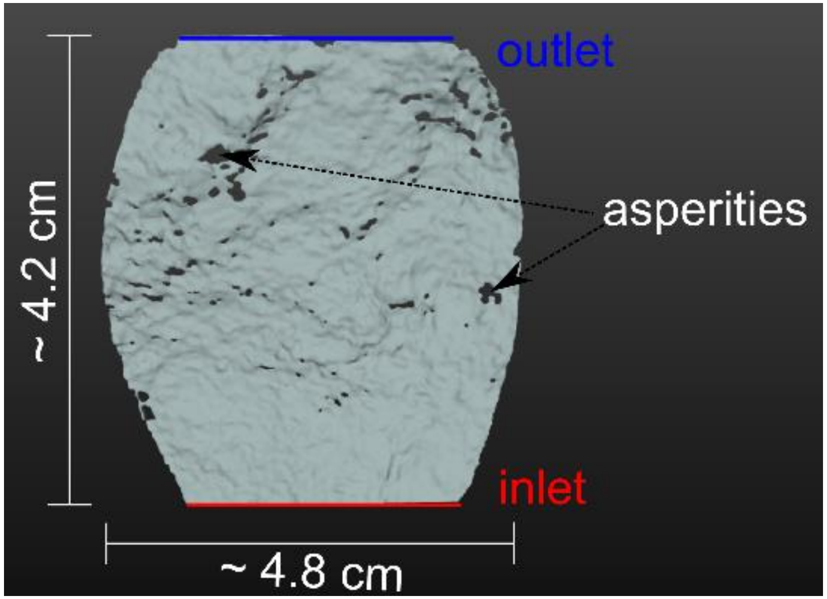
Status:

- Scan printed flow cell with µCT to verify success of printing
- If successful, prepare cell for colloid transport and bentonite erosion experiments
- Optimize design of models if necessary
- Simulation of transport experiments

Bentonite erosion in natural fractures

Bentonite erosion as f(fracture geometry)

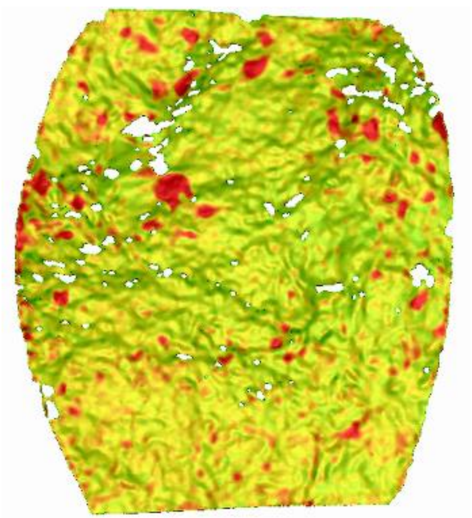
- Use of VTT erosion model (based on KTH model)
- Implemented into a 2D fracture (midplane) model
- 2 types of flow types considered:
  - Cubic Law using the aperture distribution of the fracture (by µCT)
  - Navier-Stokes flow (no apertures used)



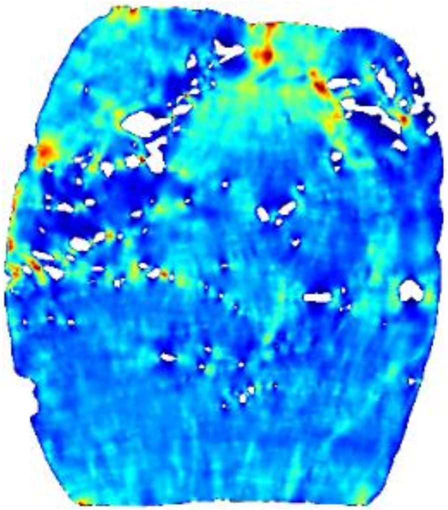
Bentonite erosion as f(fracture geometry)

- Use of VTT erosion model (based on KTH model)
- Implemented into a 2D fracture midplane model
- 2 types of flow types considered:
  - Darcy Law using the aperture distribution of the fracture (by µCT)
  - Navier-Stokes flow (no apertures used)

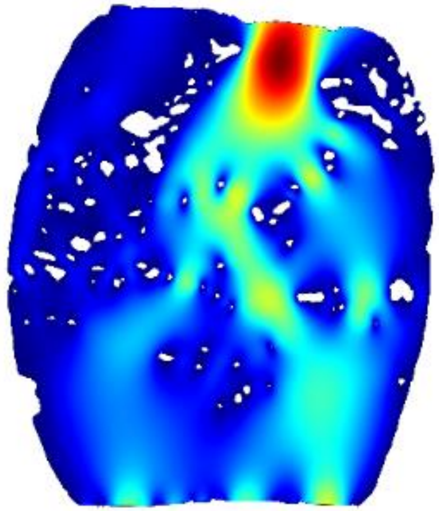
Aperture distribution



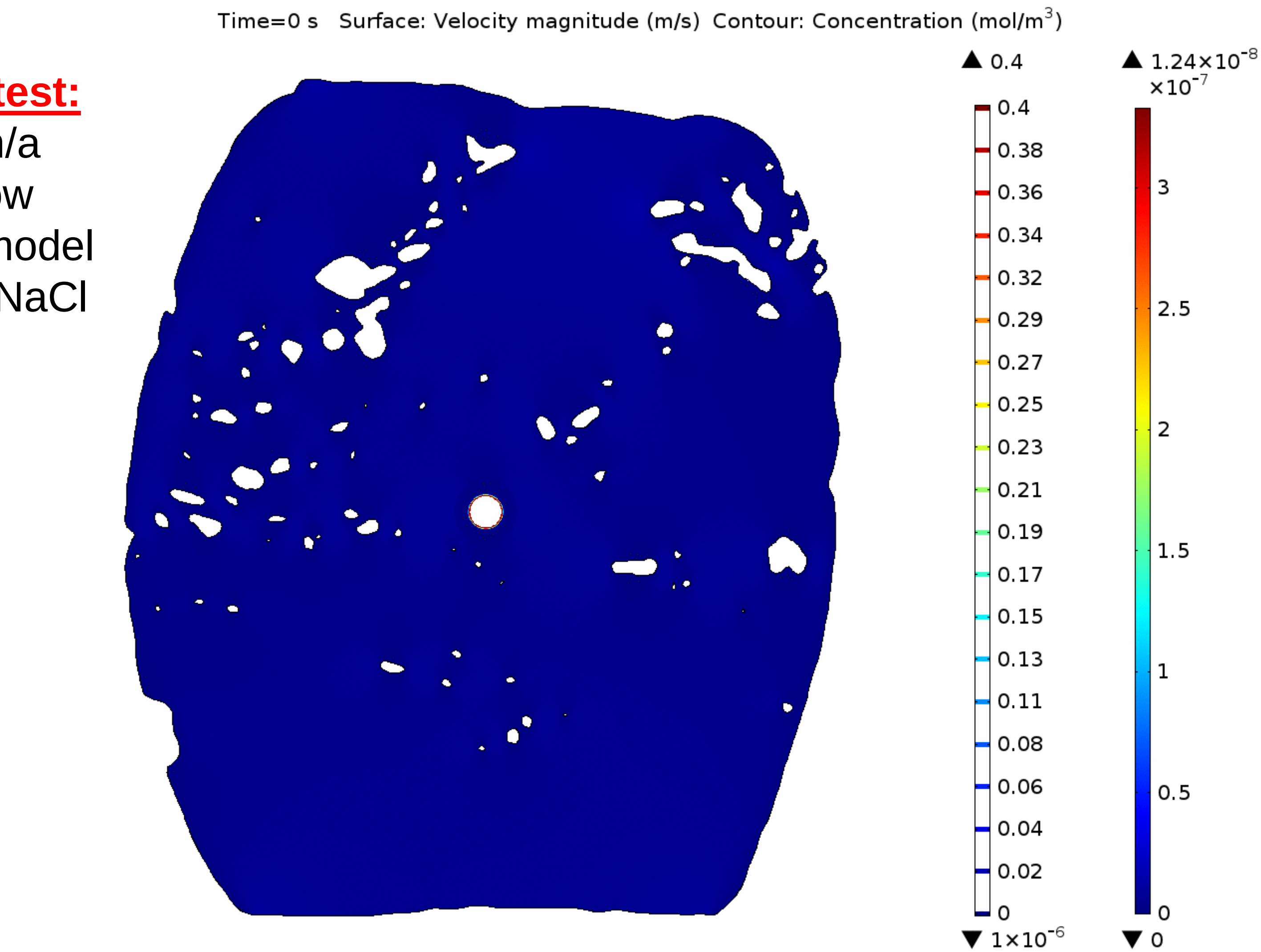
2D Darcy Law



2D Navier-Stokes



Bentonite erosion as f(fracture geometry)



First test:

3.15m/a

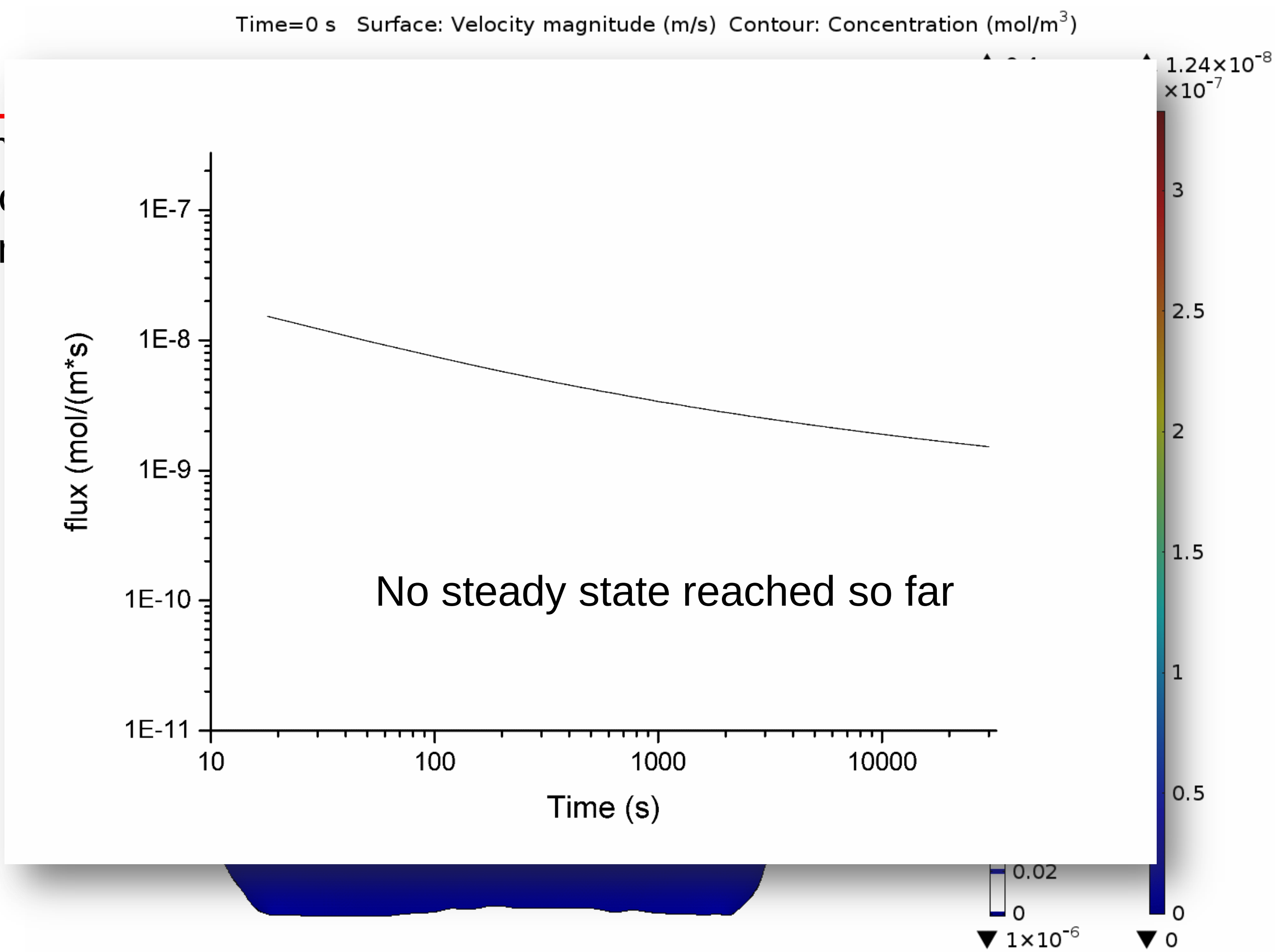
NS flow

VTT model

0.1M NaCl

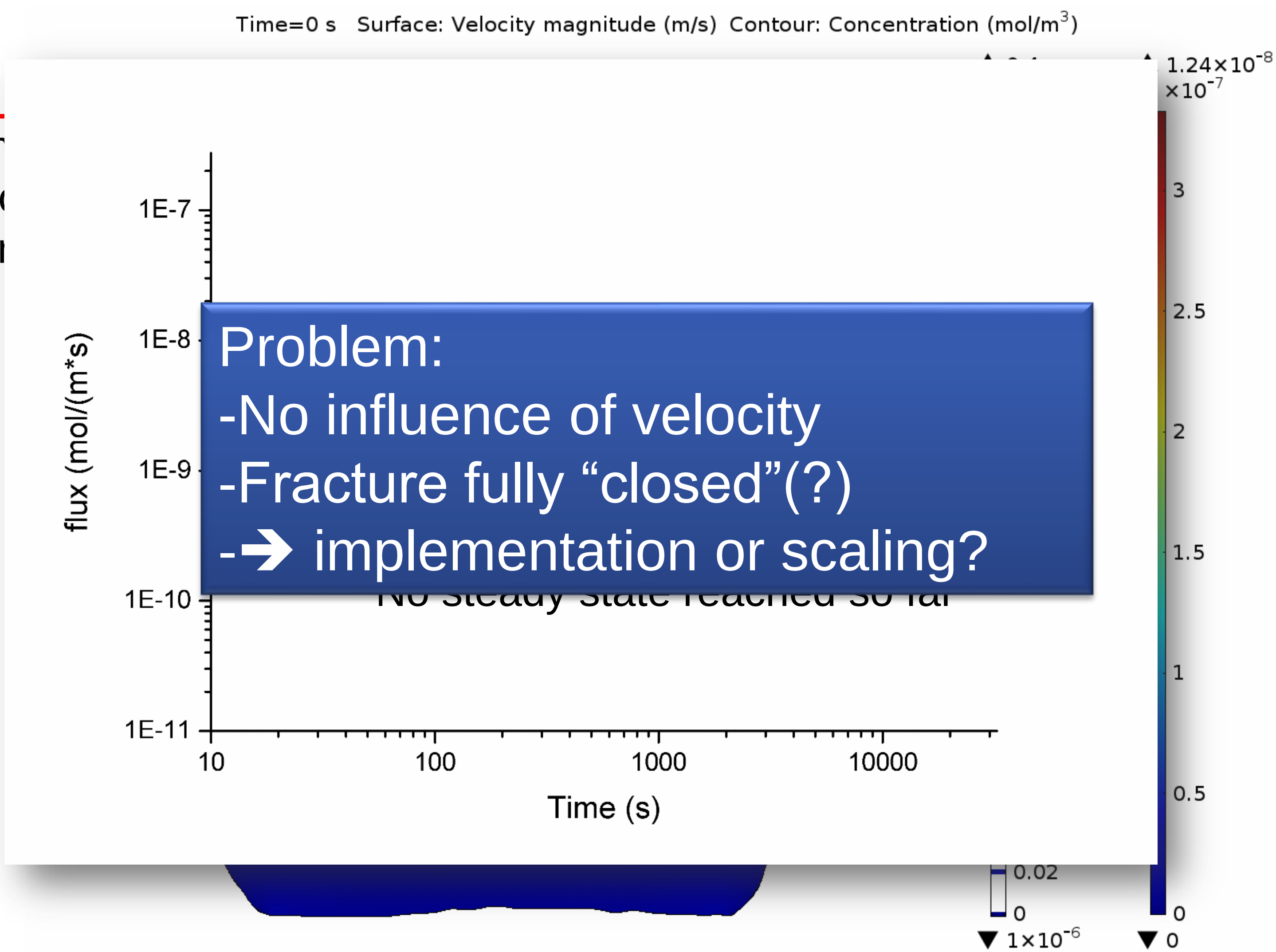
Bentonite erosion as f(fracture geometry)

First
3.15r
NS fl
VTT r
0.1M



Bentonite erosion as f(fracture geometry)

First
3.15r
NS fl
VTT r
0.1M



Problem:
-No influence of velocity
-Fracture fully “closed”(?)
-➔ implementation or scaling?

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Thanks for you attention!