Status update of the modelling work

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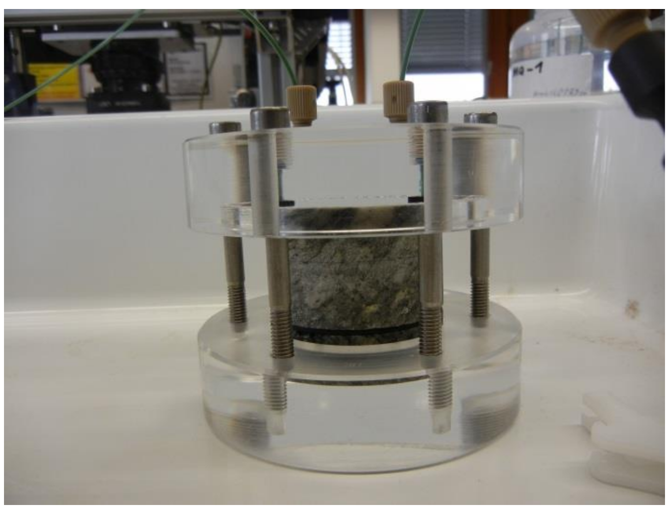

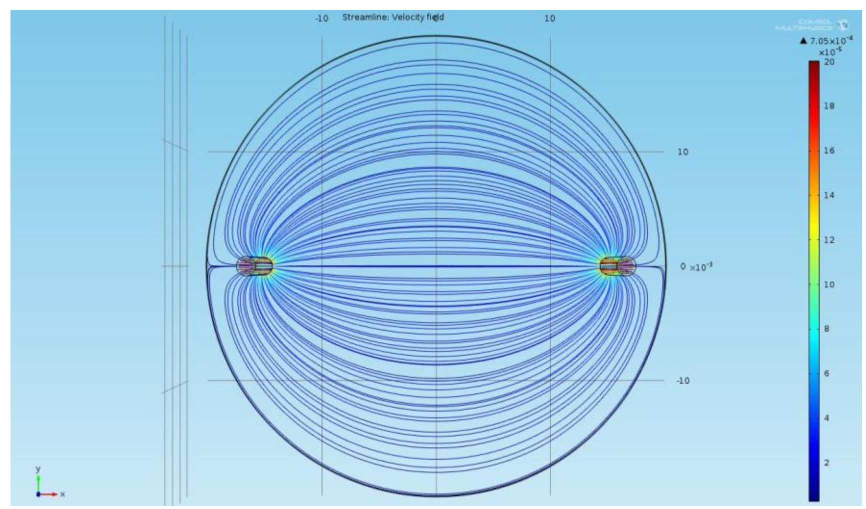

KIT-INE WP5 activities within BELBaR

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

a) Use of 3D natural fracture flow fields and 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 flow model to KTH and/or VTTs „simplified“ erosion model.
Need to consider alternative/simplified approach......

c) Colloid transport in synthetic fractures (“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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c) Colloid transport in synthetic fracture flow cell

Karlsruhe Institute of Technology

Background:

Colloid attachment has been observed under unfavorable conditions*

Reasons: surface charge heterogeneity, nanoscale fracture roughness, …

Aim: Study the impact of nanoscale fracture roughness on colloid migration

Experimental program on colloidal transport in artificial fracture flow cells (WP 3; G. Darbha)

- Conditions/parameters to be studied/varied:
  - ❖ Plexiglas "dummy" instead of granite cell to optimize setup
  - ❖ Grimsel granodiorite "fracture"
  - ❖ Grimsel ground water (pH 9.7; I = ~1e-3 M)
  - ❖ Aperture
  - ❖ Flow rate
  - ❖ Colloids: Quantum dots, (labeled) clay/bentonite, …
  - ❖ Metal ions: e.g. Eu^{3+}

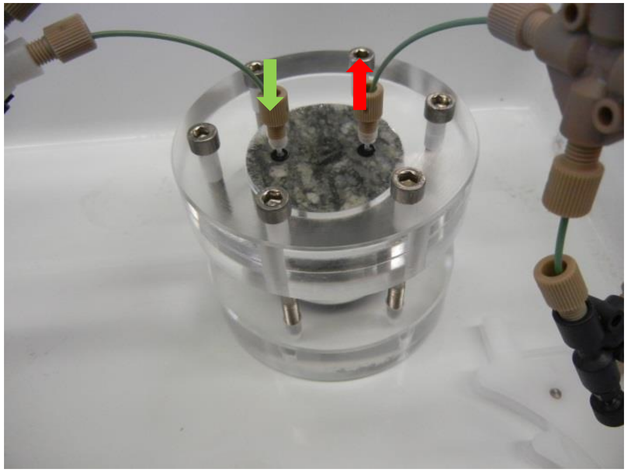
Ultimately, flow cell experiments are planned be coupled to ring erosion experiments

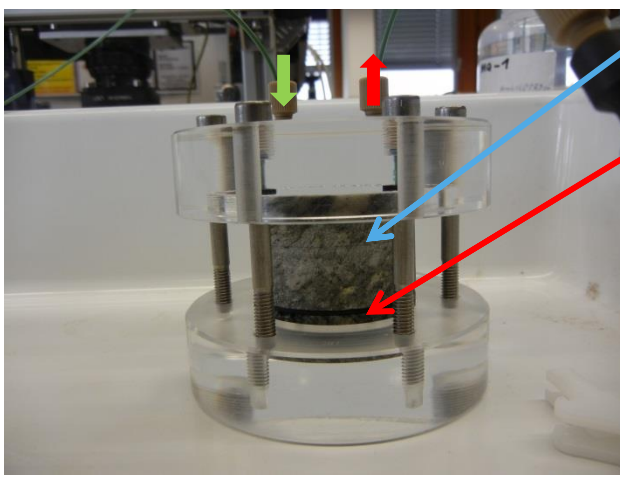
➔ freshly eroded bentonite colloids will be used

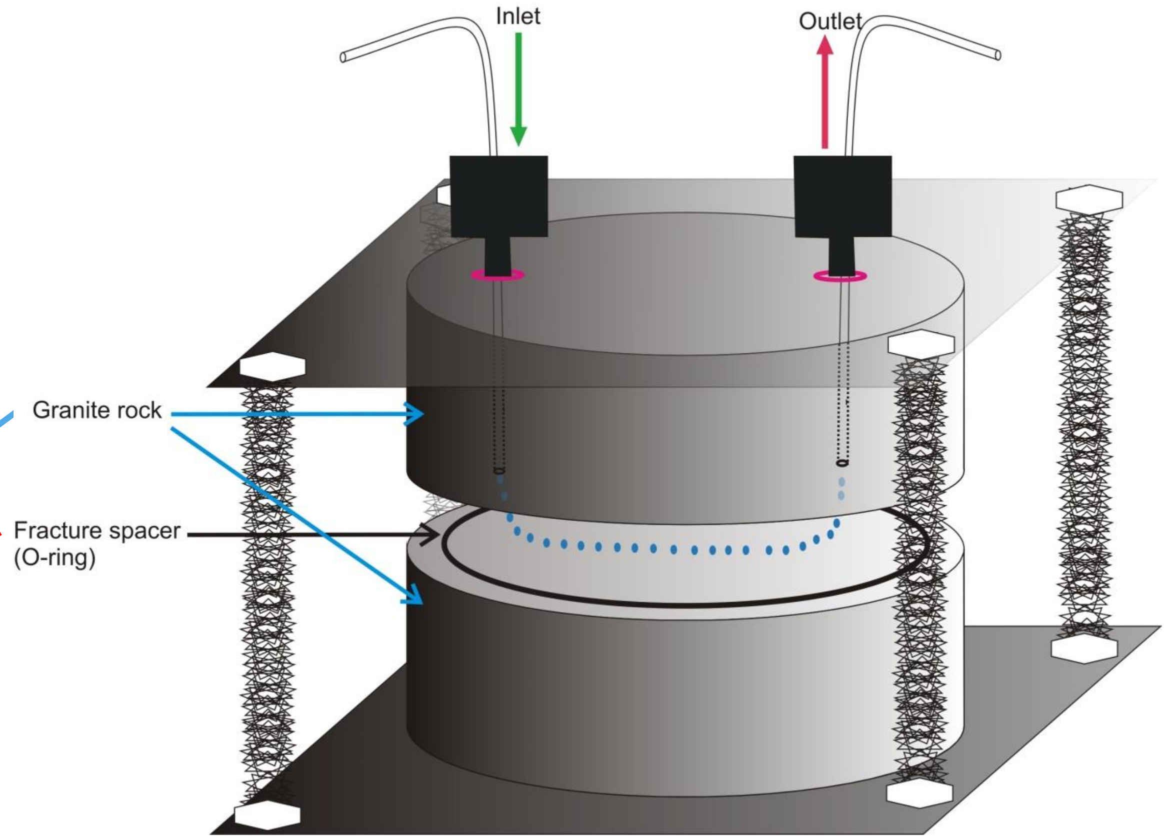
*GK Darbha, C Fischer, J Luetzenkirchen, T Schäfer. Environmental Science & Technology 46 (17)

c) Colloid transport in synthetic fracture flow cell

Fluid cell design







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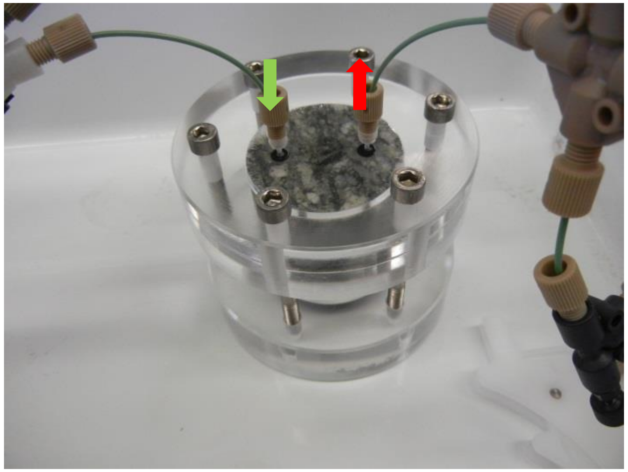
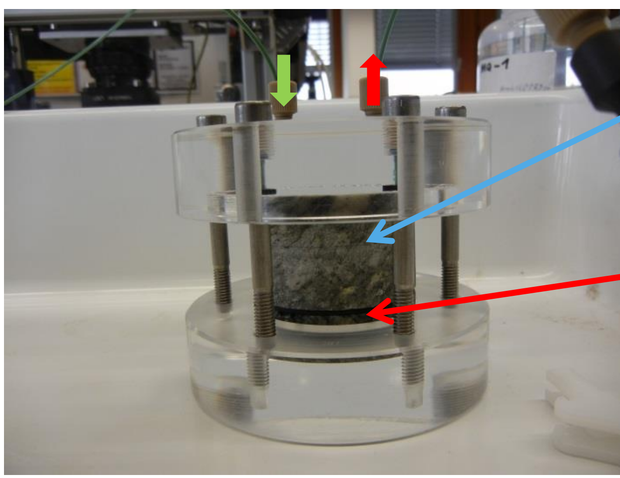
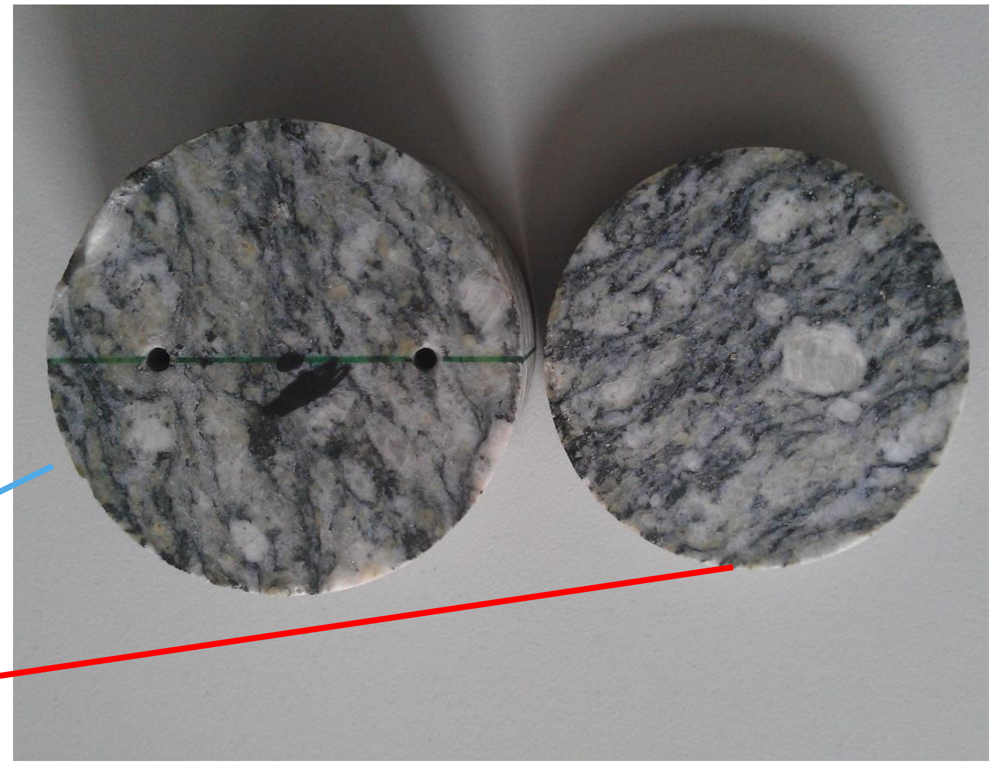
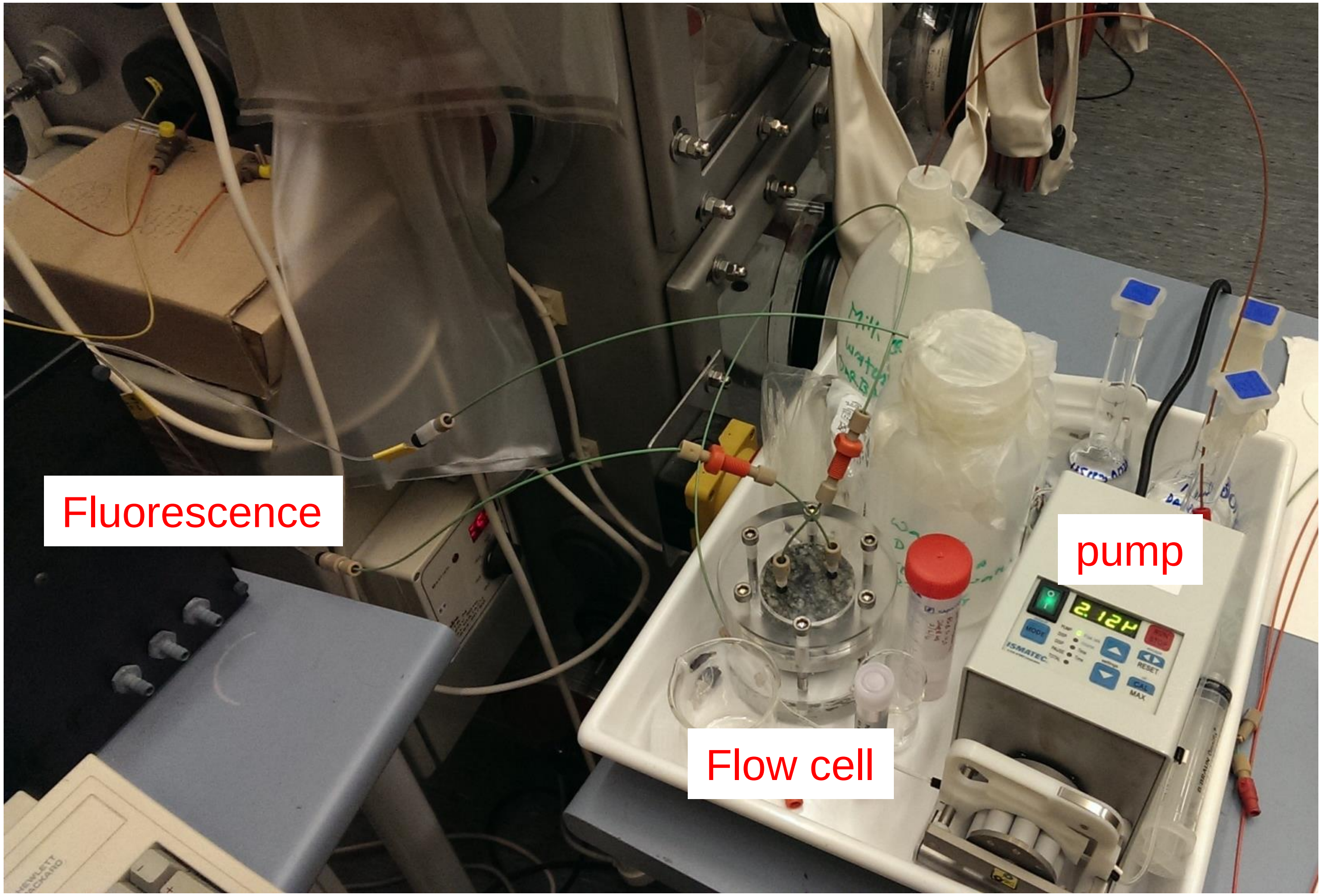
Fluid cell design #1







c) Colloid transport in synthetic fracture flow cell



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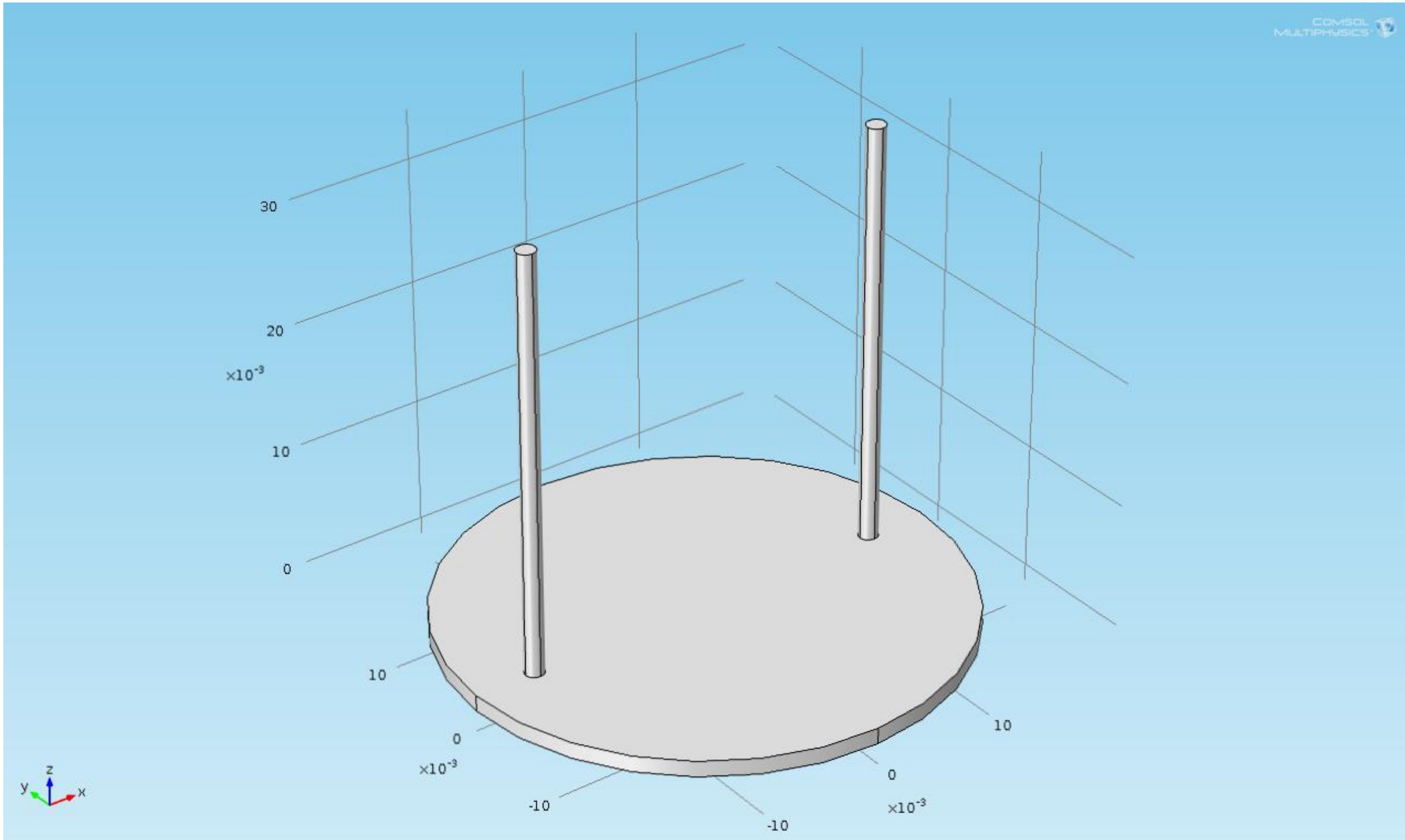
Modelling approach:

- COMSOL Multiphysics and/or ANSYS Fluent
- 3D
- Laminar, steady state, incompressible flow (Navier-Stokes)
- Solute transport modelling of inert (fluorescence) tracers (e.g. Amino-g and/or Rhodamin-b) to verify hydrodynamics
- Lagrangian Particle tracking to model colloid transport
  - ❖ Drag and lift forces, gravity, Brownian motion
  - ❖ shape correction factor due to non-spherical shape of colloids
  - ❖ exp. colloidal size distributions (bimodal, multimodal)
  - ❖ Different attachment probabilities/collision efficiencies ***α*** (that is, every x^{th} hit of the wall will led to sorption (irreversible) e.g. Grolimund et al. 2001*) of colloids for different mineral phases :
    - ➢ segmentation of fracture surface mineral distribution
    - ➢ AFM derived ***α´s*** as wall conditions for colloids,

=> surface roughness & mineralogy/chemistry is treated in this way indirectly

**Grolimund et al. / Colloids and Surfaces A: Physicochem. Eng. Aspects 191 (2001) 179–188*

c) Colloid transport in synthetic fracture flow cell



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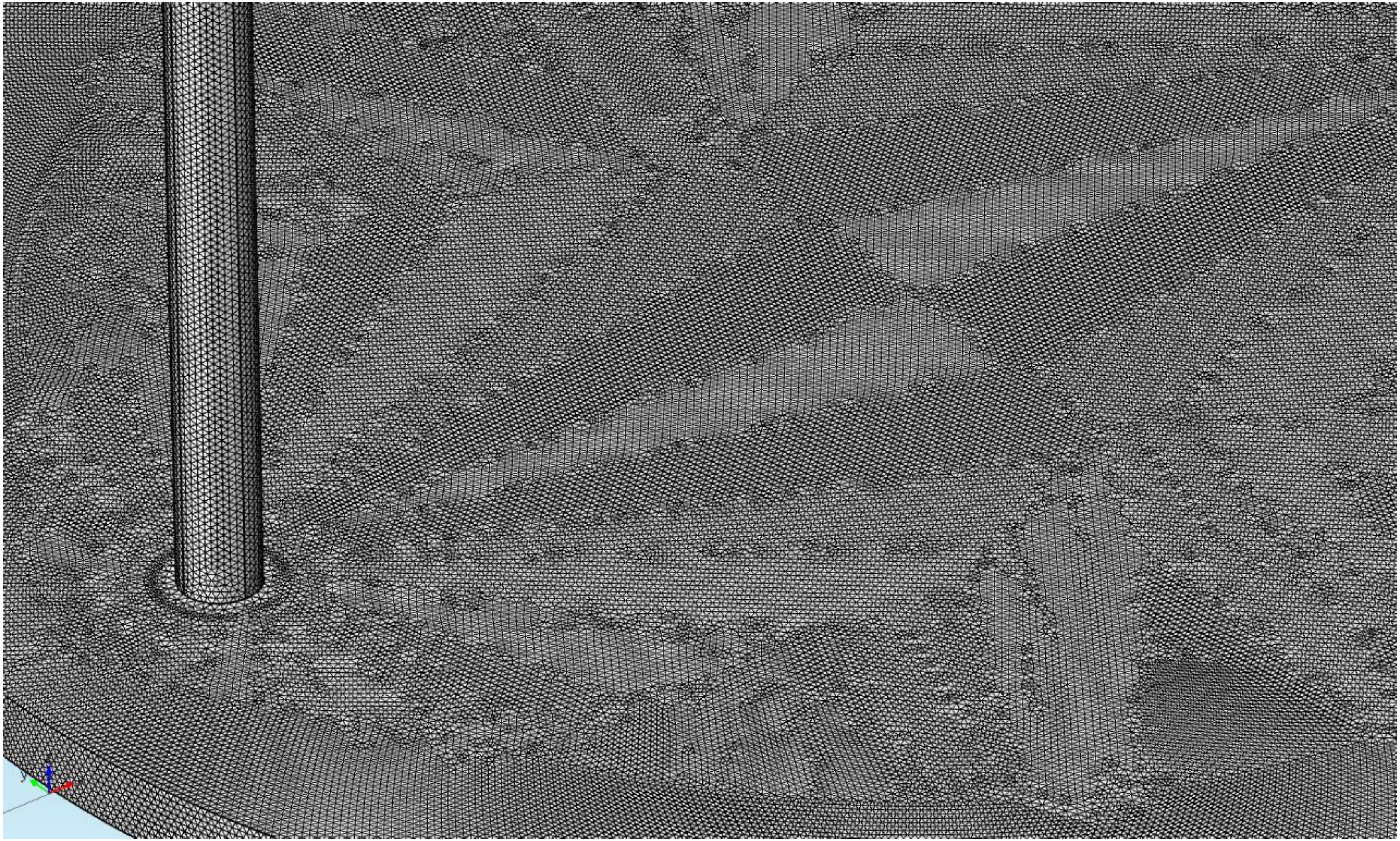

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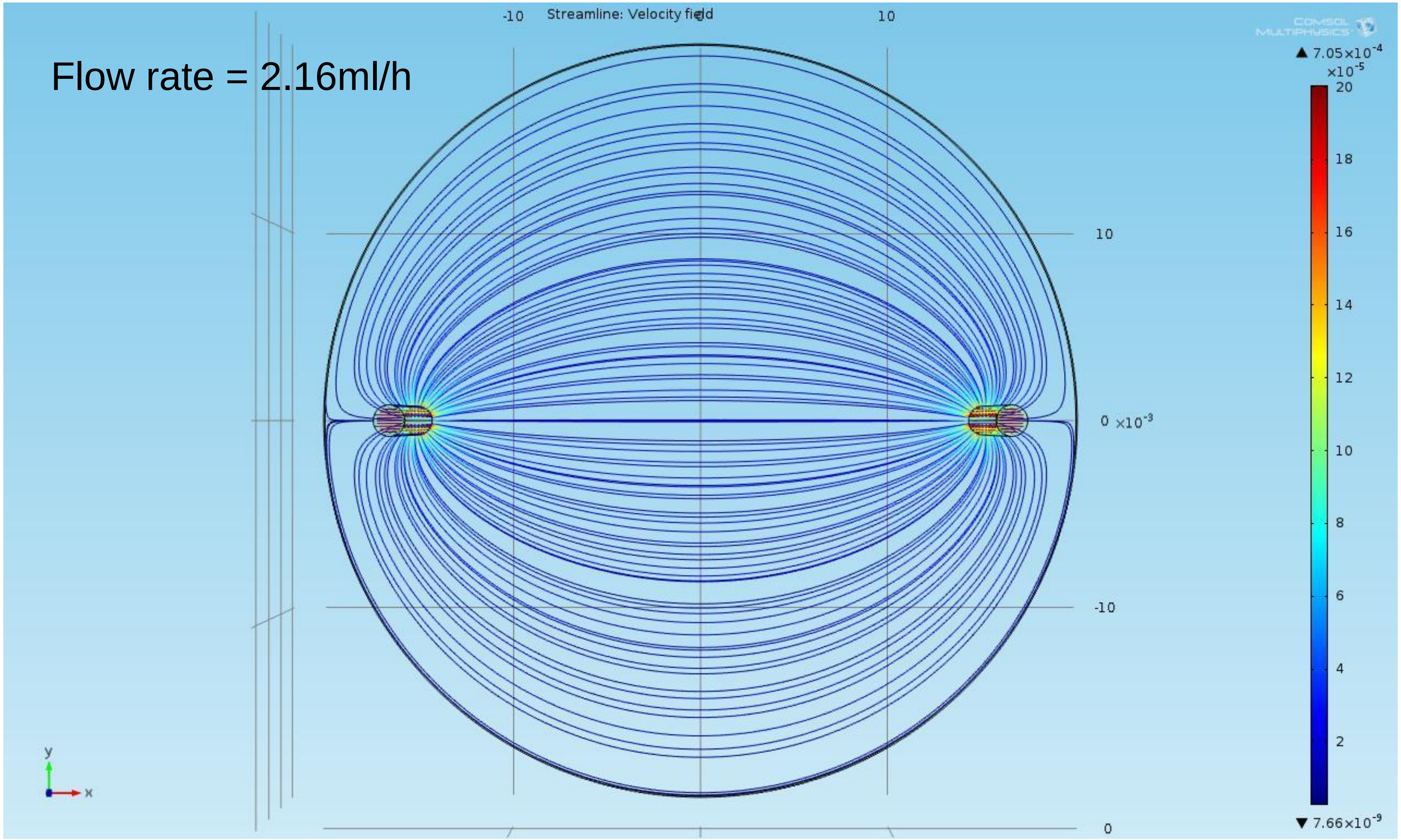
Flow rate = 2.16ml/h



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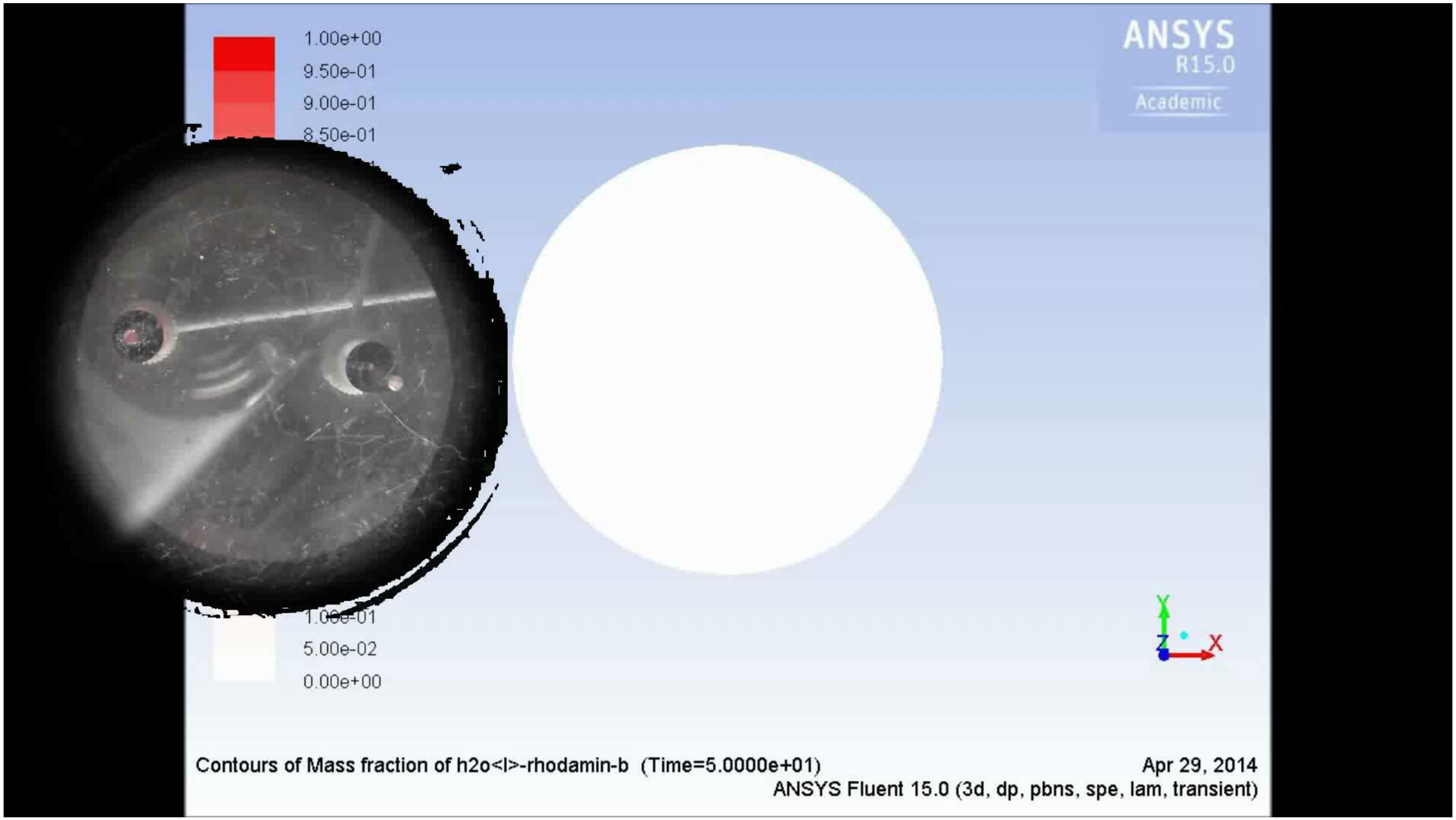

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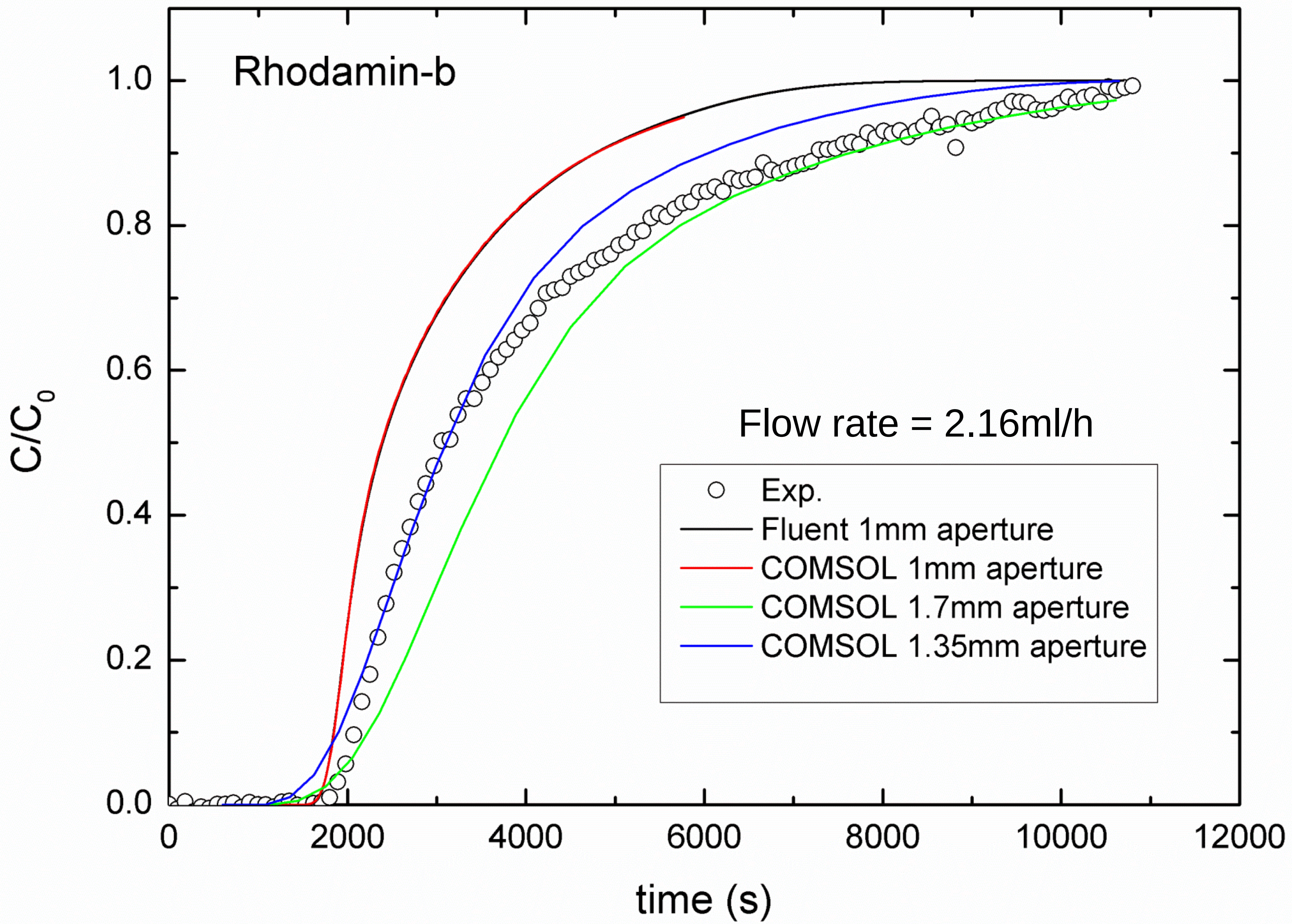
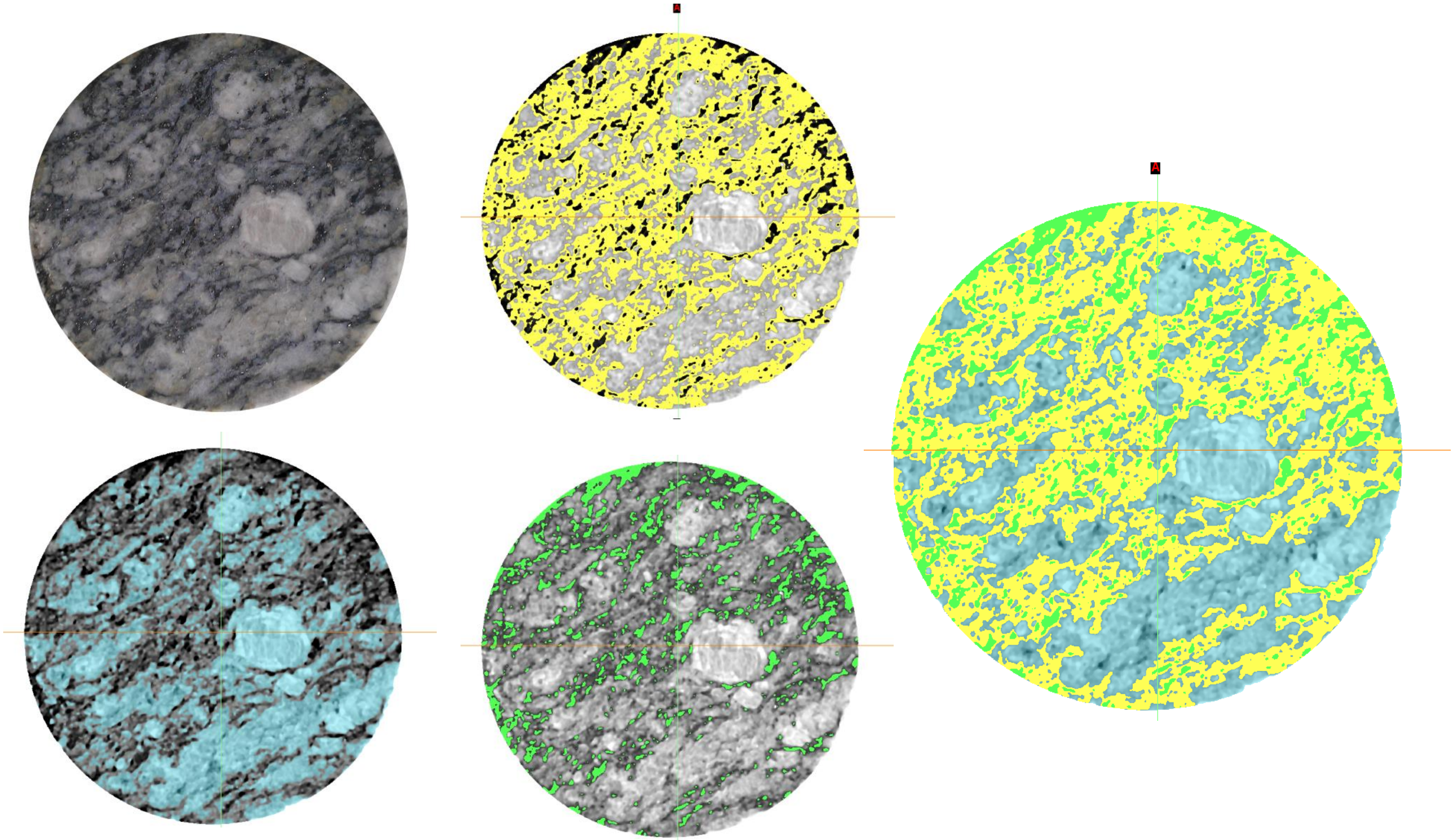


c) Colloid transport in synthetic fracture flow cell

➢Threshold segmentation of mineral phases (using Mimics Innovation Suite)



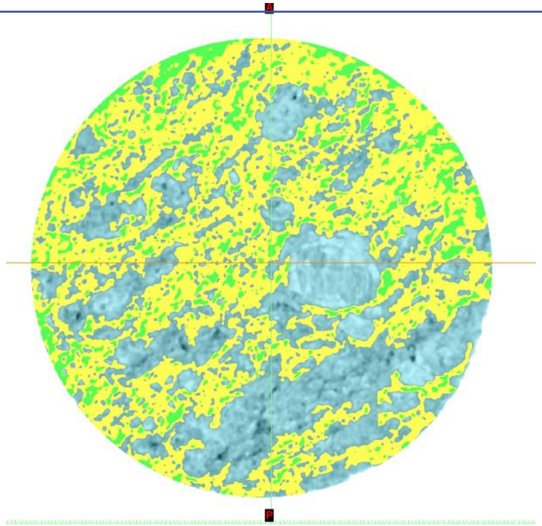
c) Colloid transport in synthetic fracture flow cell

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	Area fraction
Feldspar + Plagioclase	43.1 %
Quartz	46.9 %
„Biotite“	10 %



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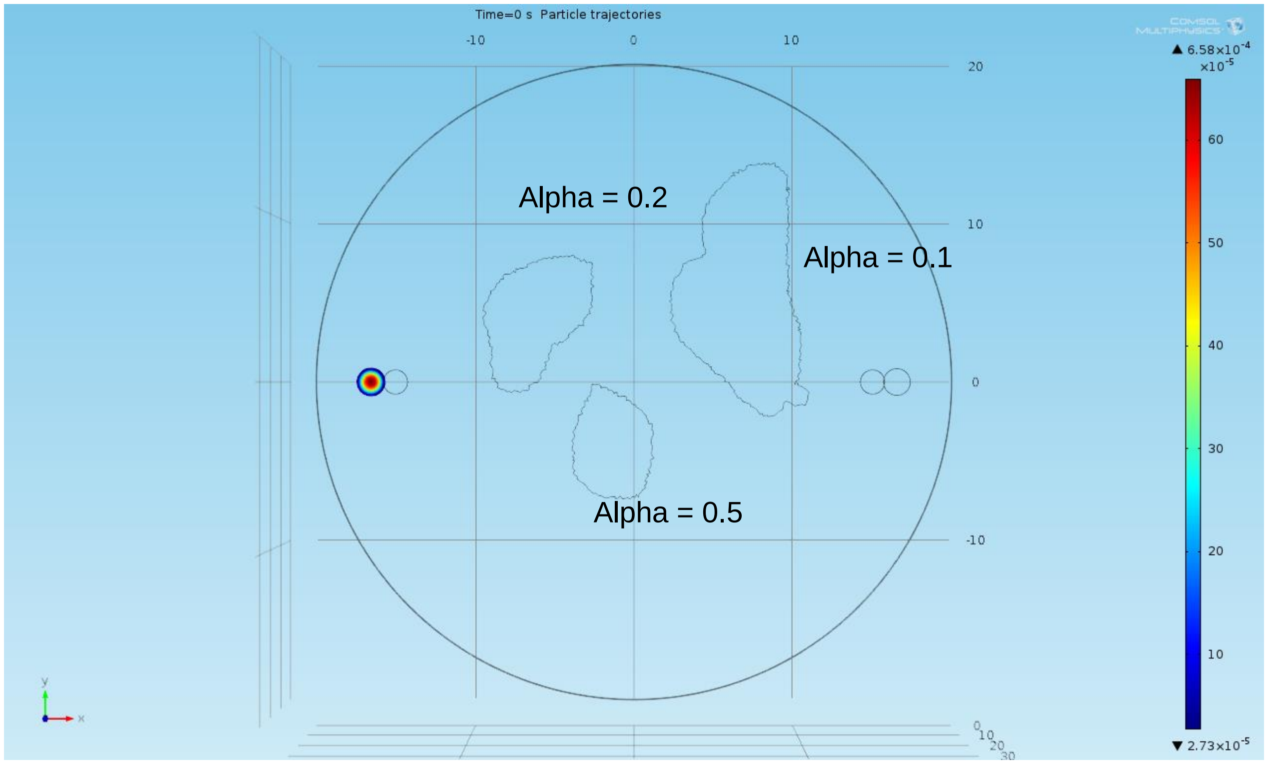
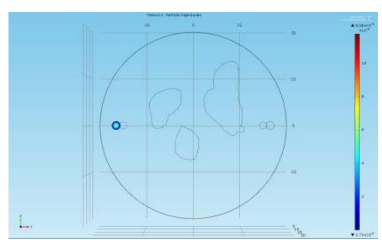
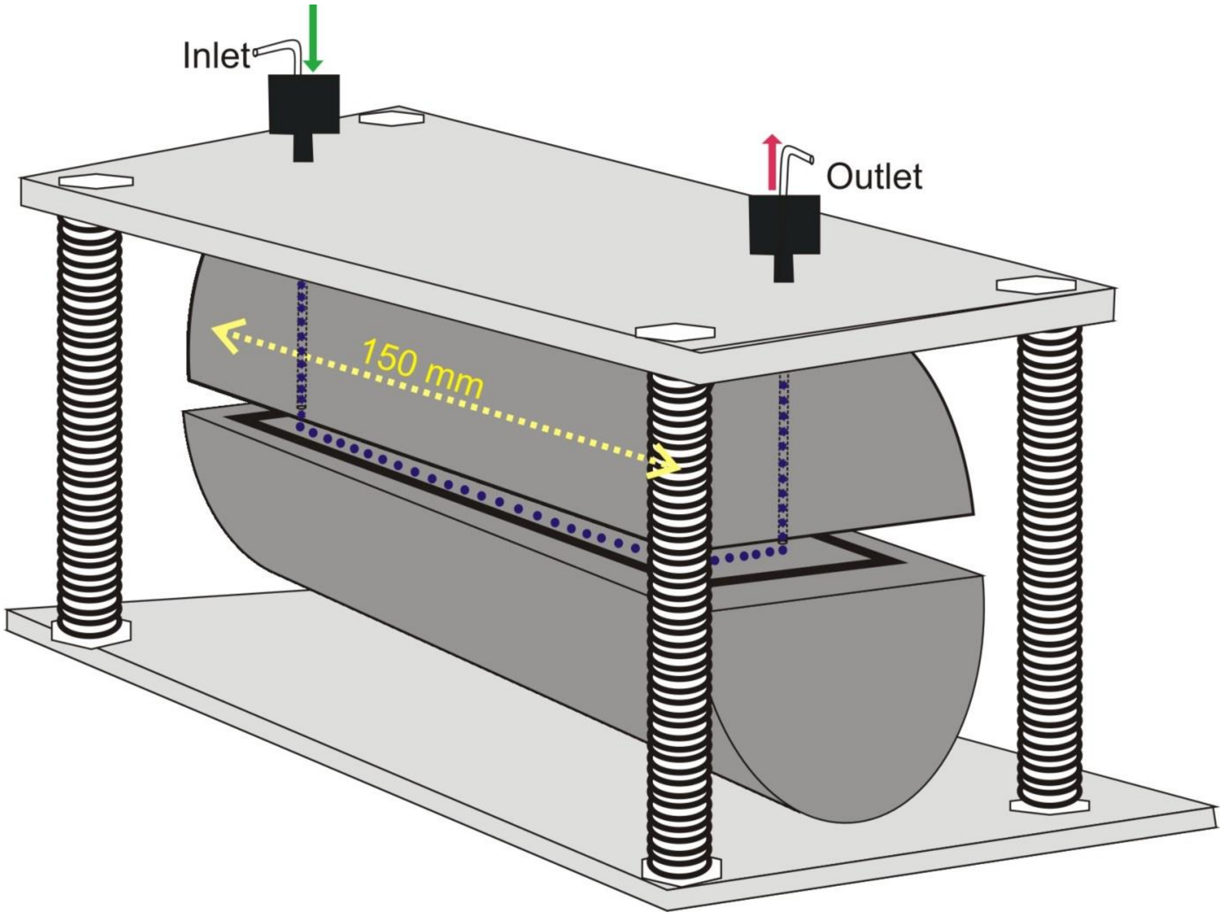




c) Colloid transport in synthetic fracture flow cell

flow cell #2



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