Business from technology

Bentonite erosion by dilute waters – some implementations of Neretnieks' model

BELBaR meeting 5-7 March 2012

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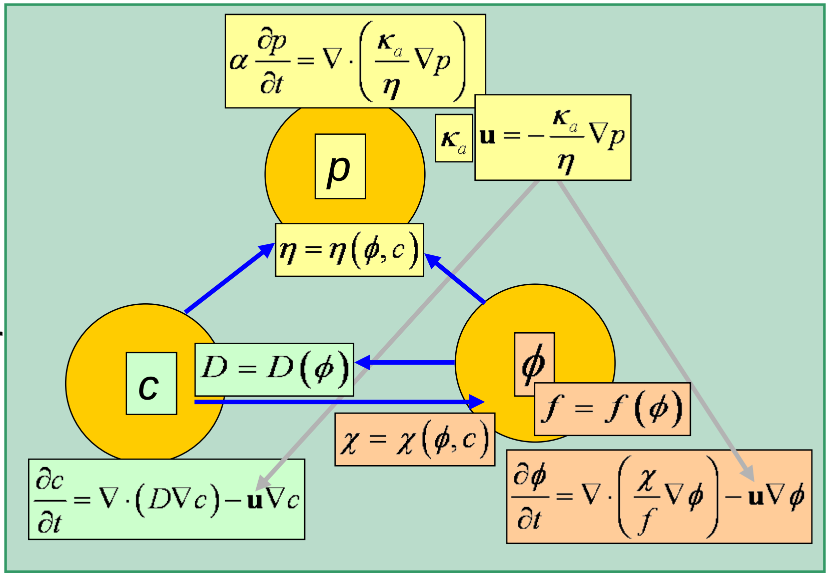
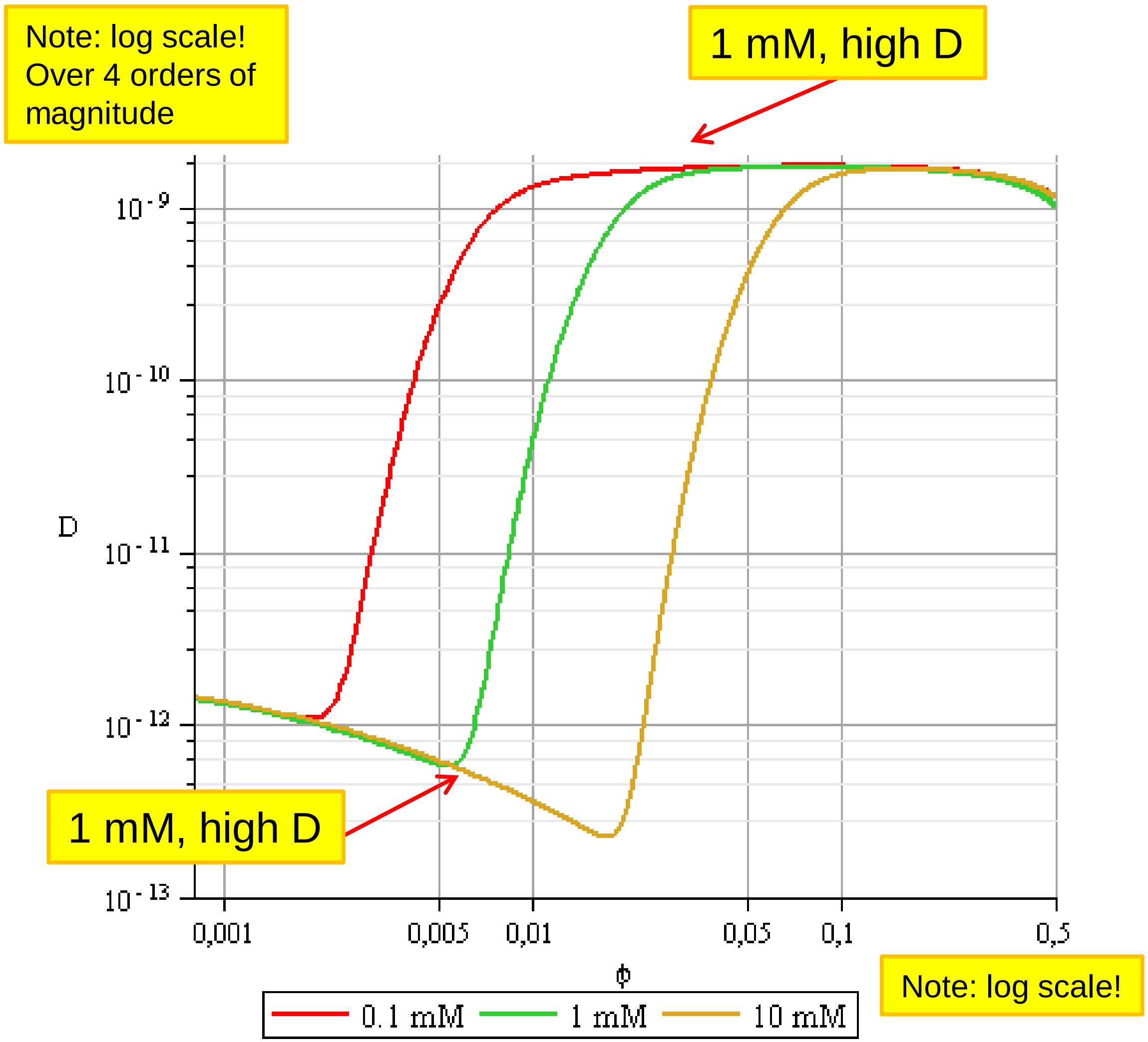
Introduction



- Job to be done
  - How to estimate the loss of buffer or filling material through contact with dilute groundwater at a transmissive fracture interface?
- Proposed solutions
  1. Modelling, SKB, Neretnieks' et al. model
  2. Experiments, Posiva, Schatz's experiments
- Impact
  - Scientific support for PA scenarios and calculations – confidence building
- Concepts
  1. Develop a model based on solid science (Neretnieks et al.) – and solve it
  2. Carry out experiments in conditions as realistic as possible (Schatz et al.)
  3. Combine all this – to be done in EU BELBaR?
- This presentation is targeted in solving Neretnieks' model and comparing it to experiment (Schatz et al.) when possible

Bentonite expands by non-linear diffusion

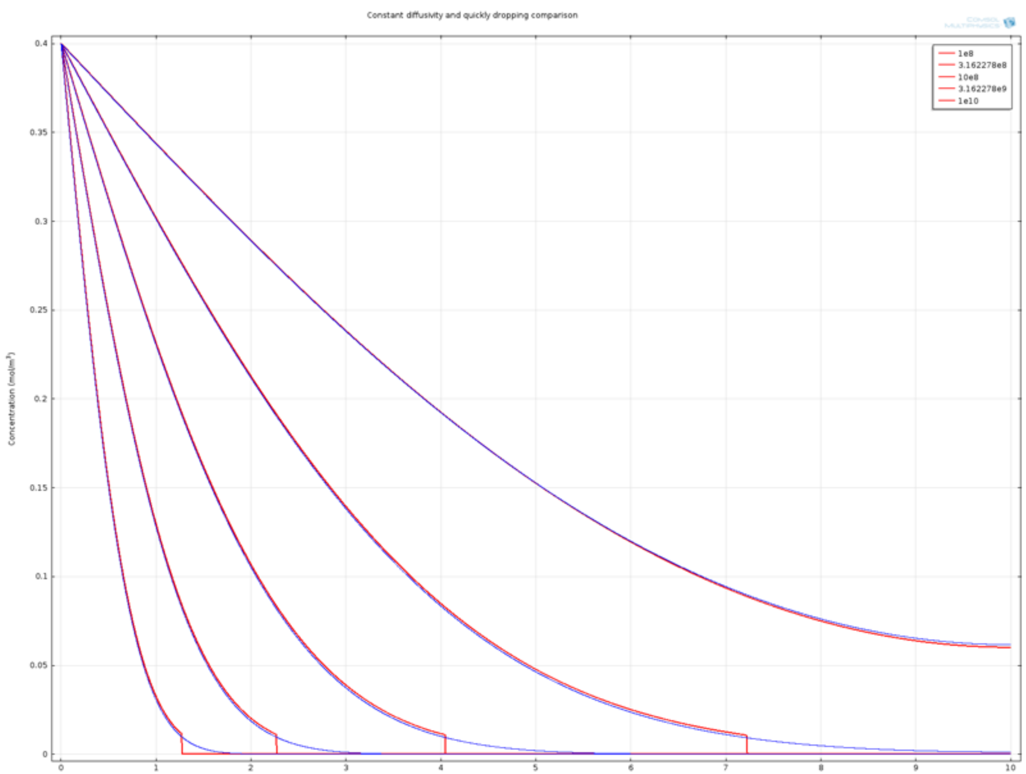


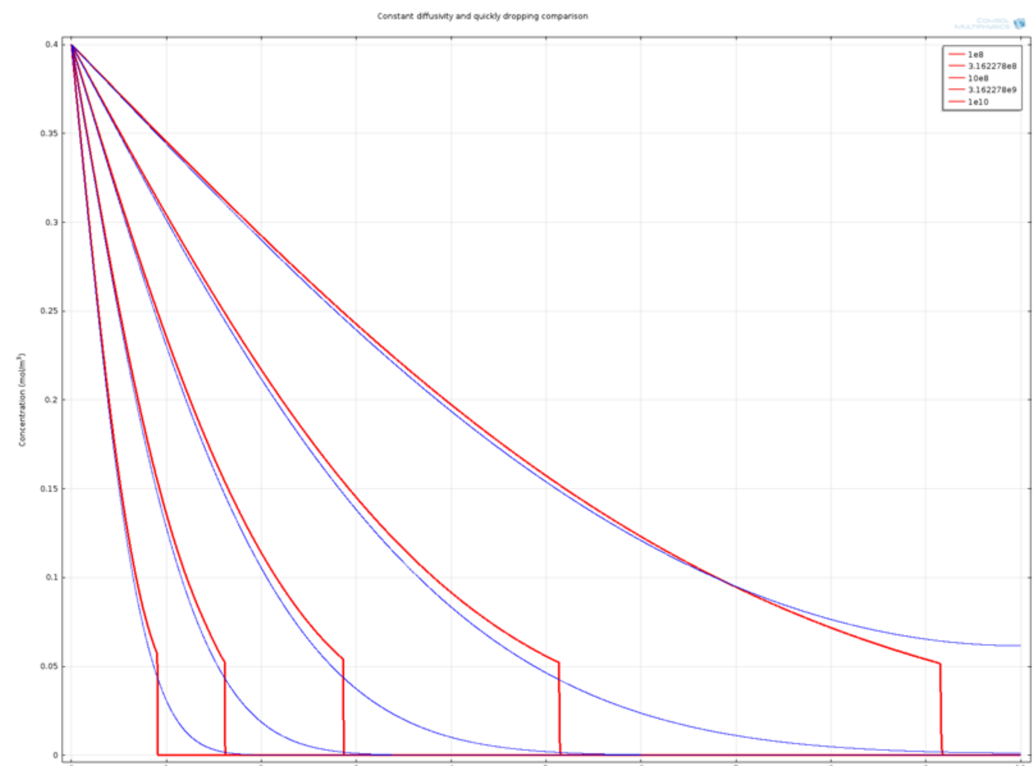
- Non-linear: diffusivity of bentonite depends on volume fraction of bentonite (or montmorillonite), ϕ
- At 1 mM solution
  1. High diffusivity (like ions in free water) above $\phi \approx 0.040$
  2. Low (more than three orders of magnitude) diffusivity under $\phi \approx 0.006$
- By decreasing salinity dropdown changes to lower values of ϕ
- However, at low ϕ values groundwater flow starts to be an important transport mechanism → erosion of bentonite

Erosion zone

Consequences of non-linear diffusivity

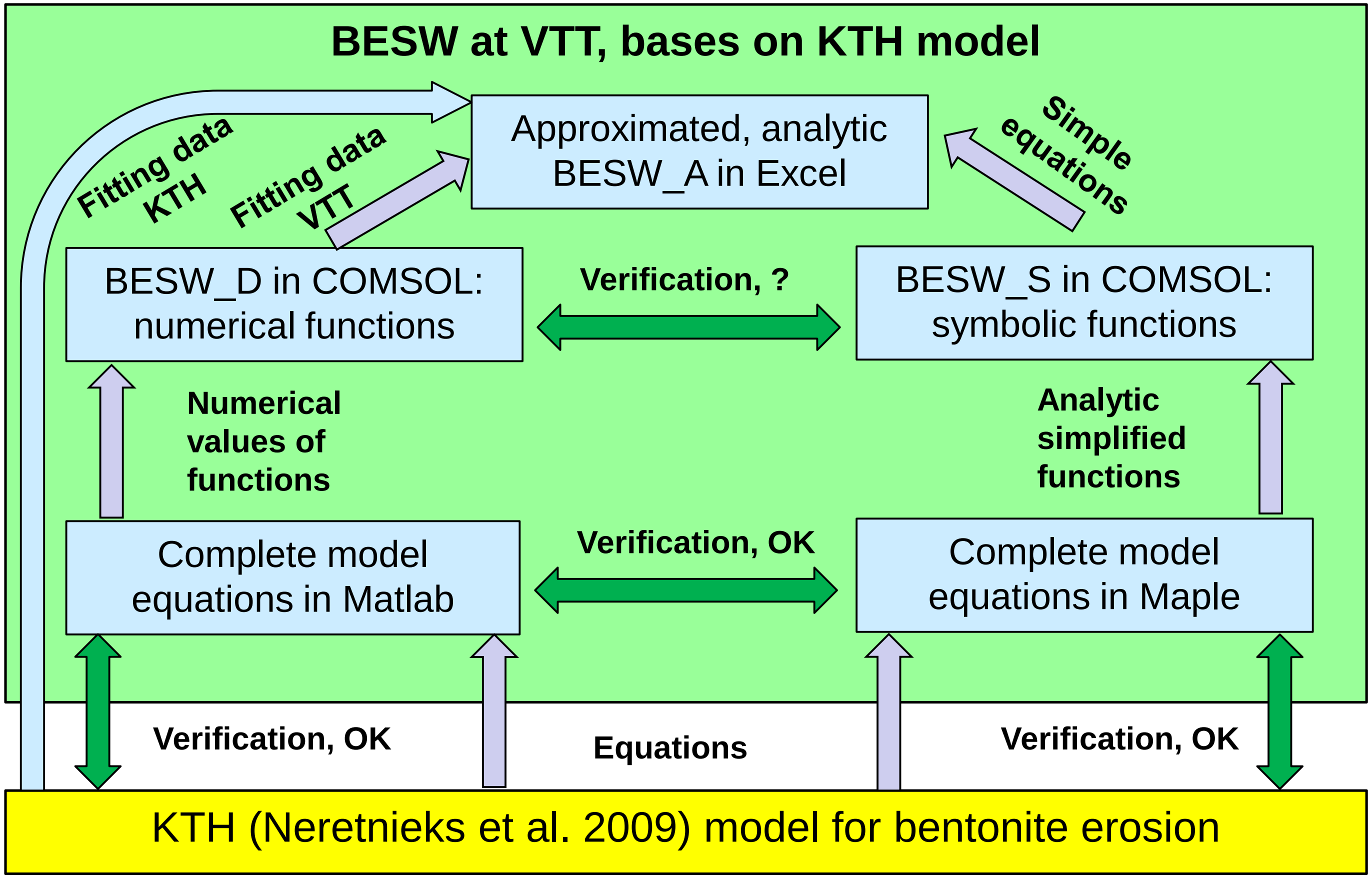
- Simple model in COMSOL Multiphysics: $D_F = D_h*(c>c_0)+D_l$
- Left cutting volume fraction 0.01 (1 mM) and right 0.05 (> 10 mM)
- Observation: overall diffusion curves are similar, but there is nothing (c=0) in the low diffusivity area
- No big difference between salinities for overall behaviour





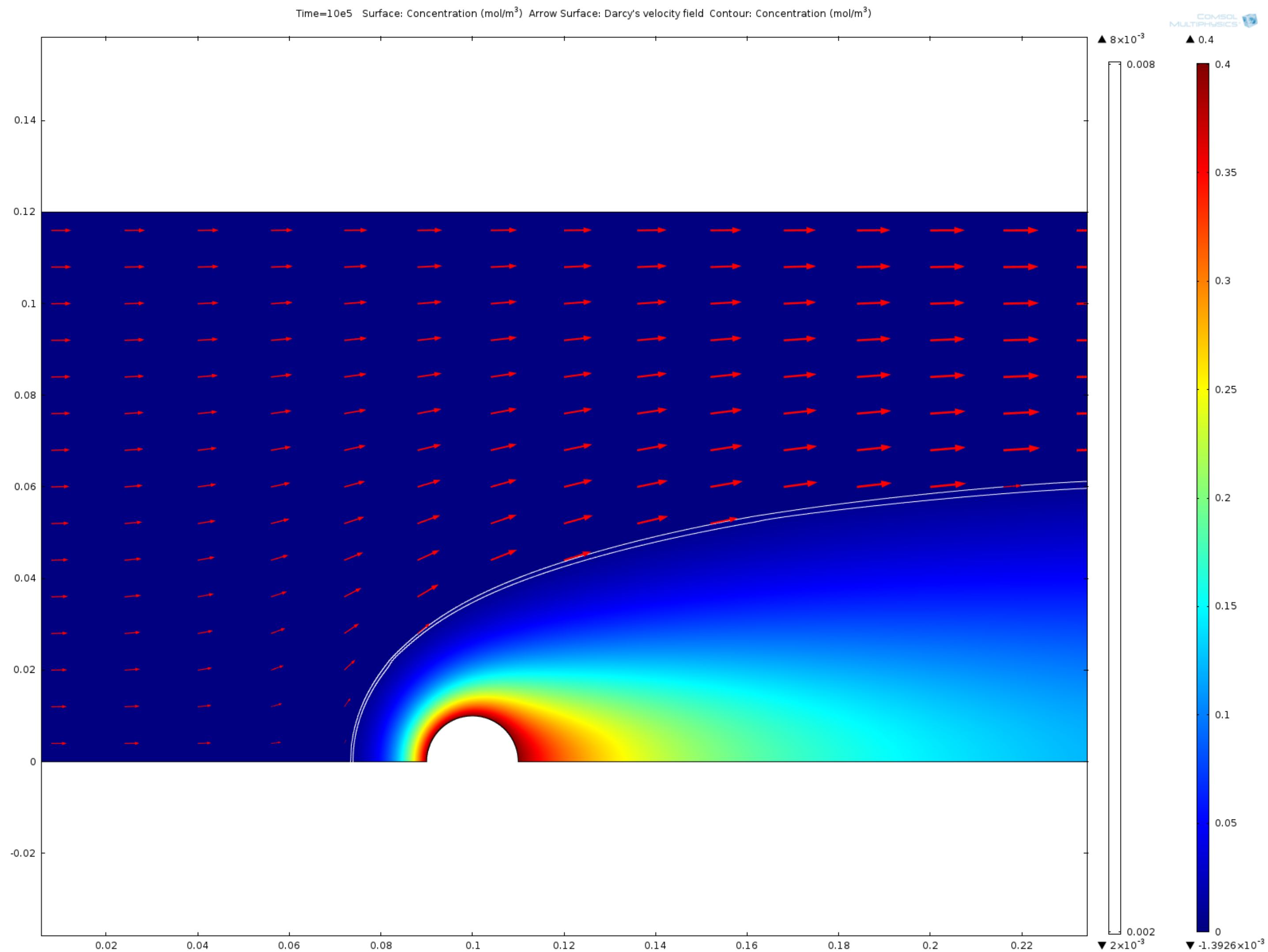
Neretnieks' model (named BESW) implementations at VTT

- BESW is complicated set of equations including several nested function calls
- Several implementations to enable verification and helping in solving



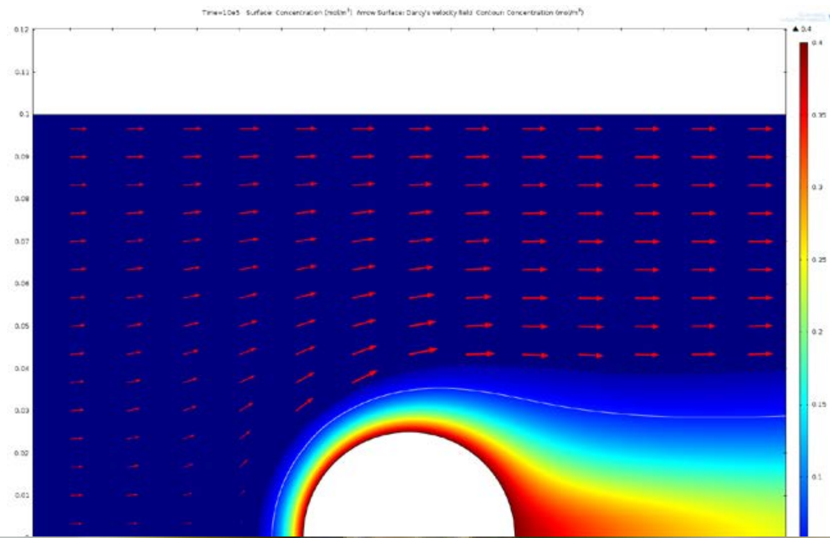
Small scale example, full

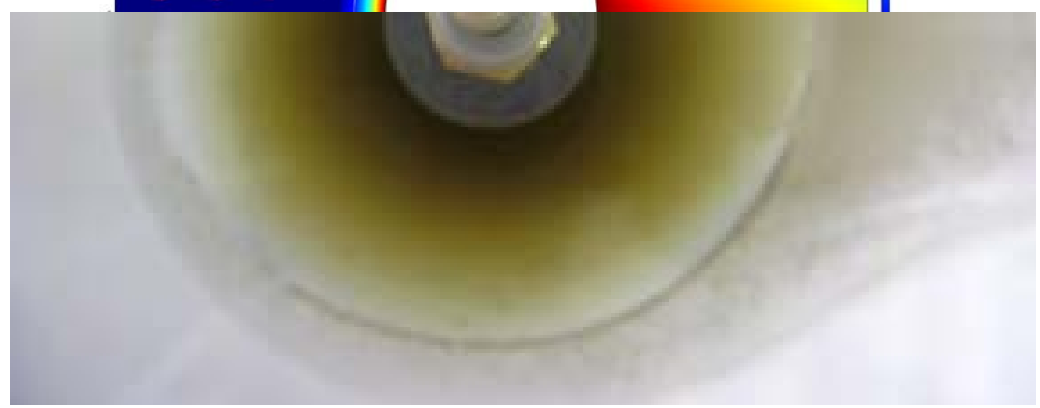
- Small scale system:
  I = 0.1 mM
  v = 2000 m/a
  R = 1 cm
  t =1e6 s
- 390 000 mesh elements, over 1.5 million DOFs
- computing time by Dell T3500, less than four days
- D_F drop 0.002 – 0.008 (contour lines)



Experiments and numerical modelling

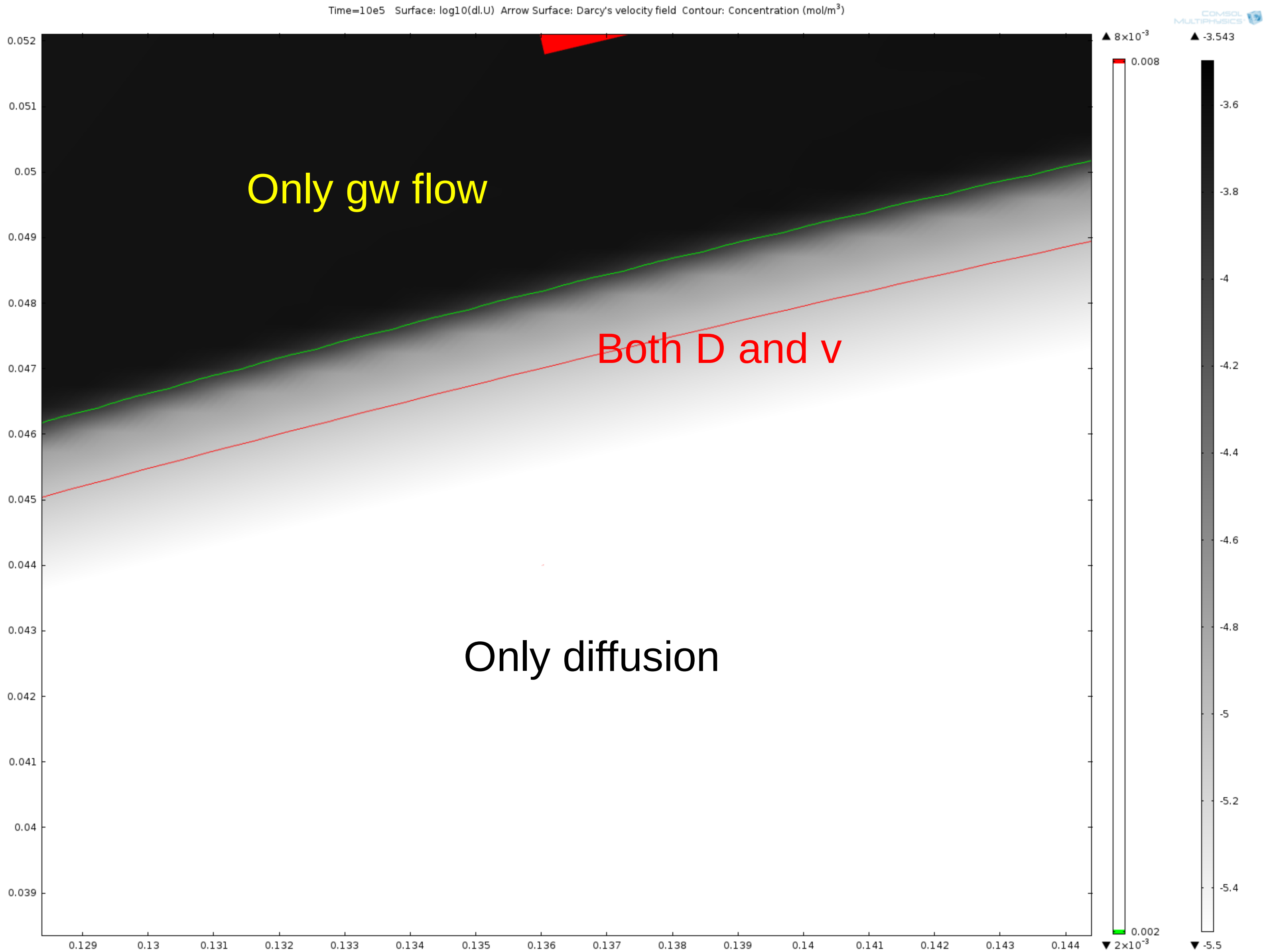
- Comparison of
  - COMSOL result by constant salinity applying our analytical formula in 2D
  - Schatz experimental observation
- Top: modelling results (volume fraction of smectite) of Neretnieks' model by COMSOL, fixed salinity of 100 µM NaCl.
- Bottom: Photo of an aperture swelling experiment (Schatz et al.), de-ionized water. Flow velocity is high at about 2 000 m/a and both images are taken about 6 days after the appearance of dilute water.
- Both the extrusion distance and shape differ, but not so much – thinking the uncertainties included





Erosion zone

- Contour lines: high and low diffusivity 0.002 and 0.008
- Surface: ground water flow velocity, log scale, two orders of magnitude



- When ϕ high, D_F high (h)
- When ϕ low, D_F low (l)
- At very low volume fraction colloidal diffusivity (c)
- Turning point as a function of volume fraction varies as a function of salinity

For testing purposes mainly: an analytic expression for D_F

Trial functions

$$D_F(\phi,c) = D_F^l \cdot \left(\frac{D_F^h}{D_F^l}\right)^{\alpha(\phi,c)} + D_F^c$$

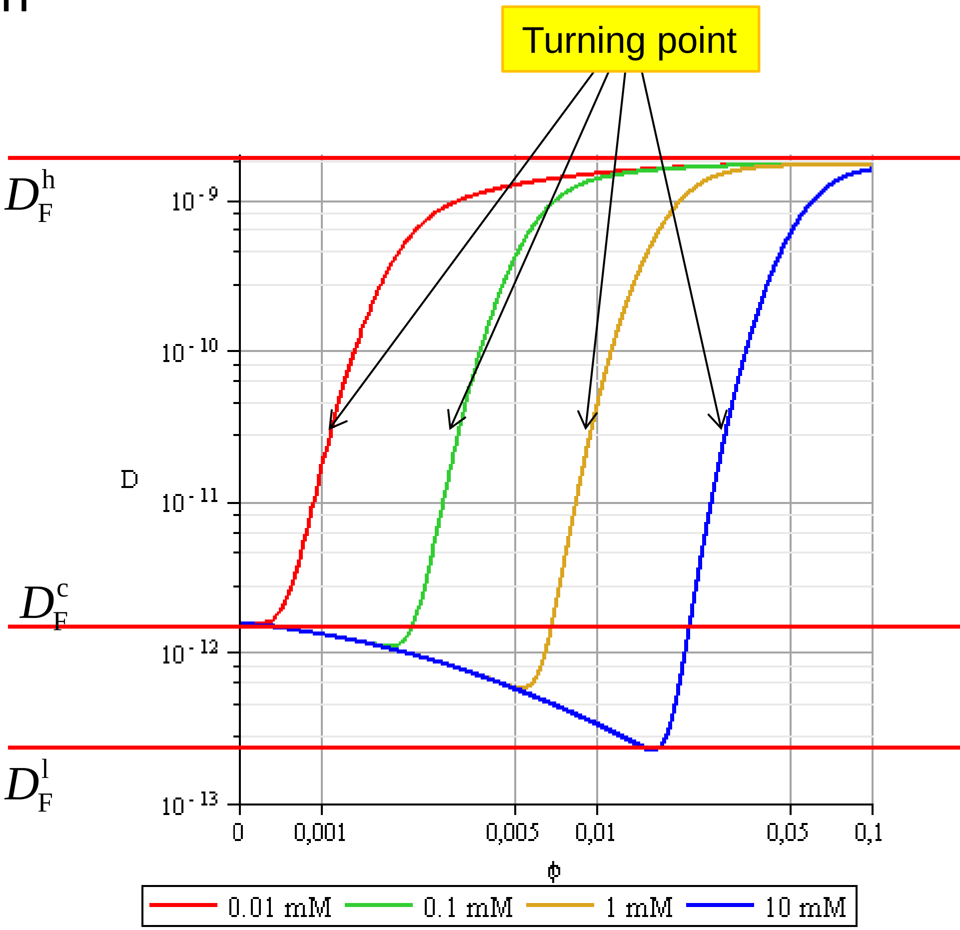
$$\alpha = \alpha(\phi,c) = \left(1 + \left(\frac{\ln\phi}{\ln\phi_{critical}}\right)^n\right)^{-1}$$

$$\phi = 1, \alpha = 1$$

$$\phi \to 0, \alpha \to 0$$

$$\phi_{turning} = Ac^b \cong 0.01\sqrt{c}$$

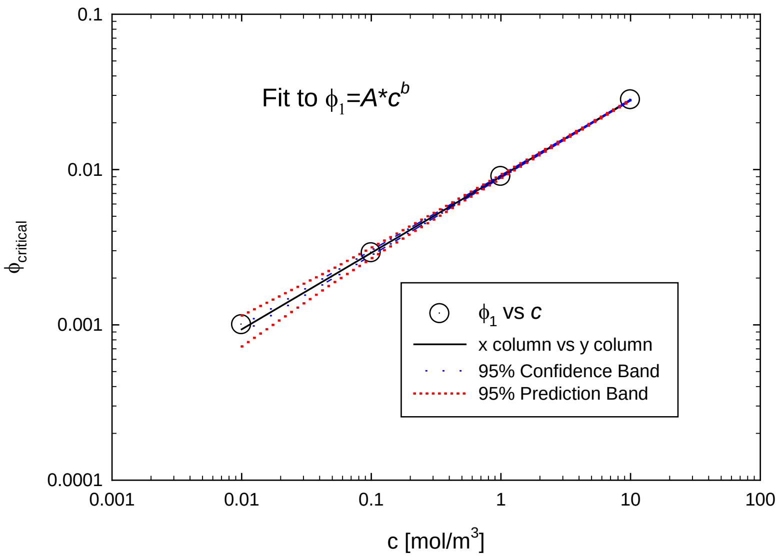
$$\alpha = \alpha(\phi,c) = \left(1 + \left(\frac{\ln\phi}{\ln A + b\ln c}\right)^n\right)^{-1}$$



Fitting parameters and goodness of fitting

- Parameters in Table and fititng in Figures

Parameter	Value	Unit
n	16	-
A	0.009± 3.90E-005	-
b	0.492± 0.0020	-
D_F^h	1.6e-9	m^2/s
D_F^l	1e-13	m^2/s
D_F^c	1.9e-12	m^2/s



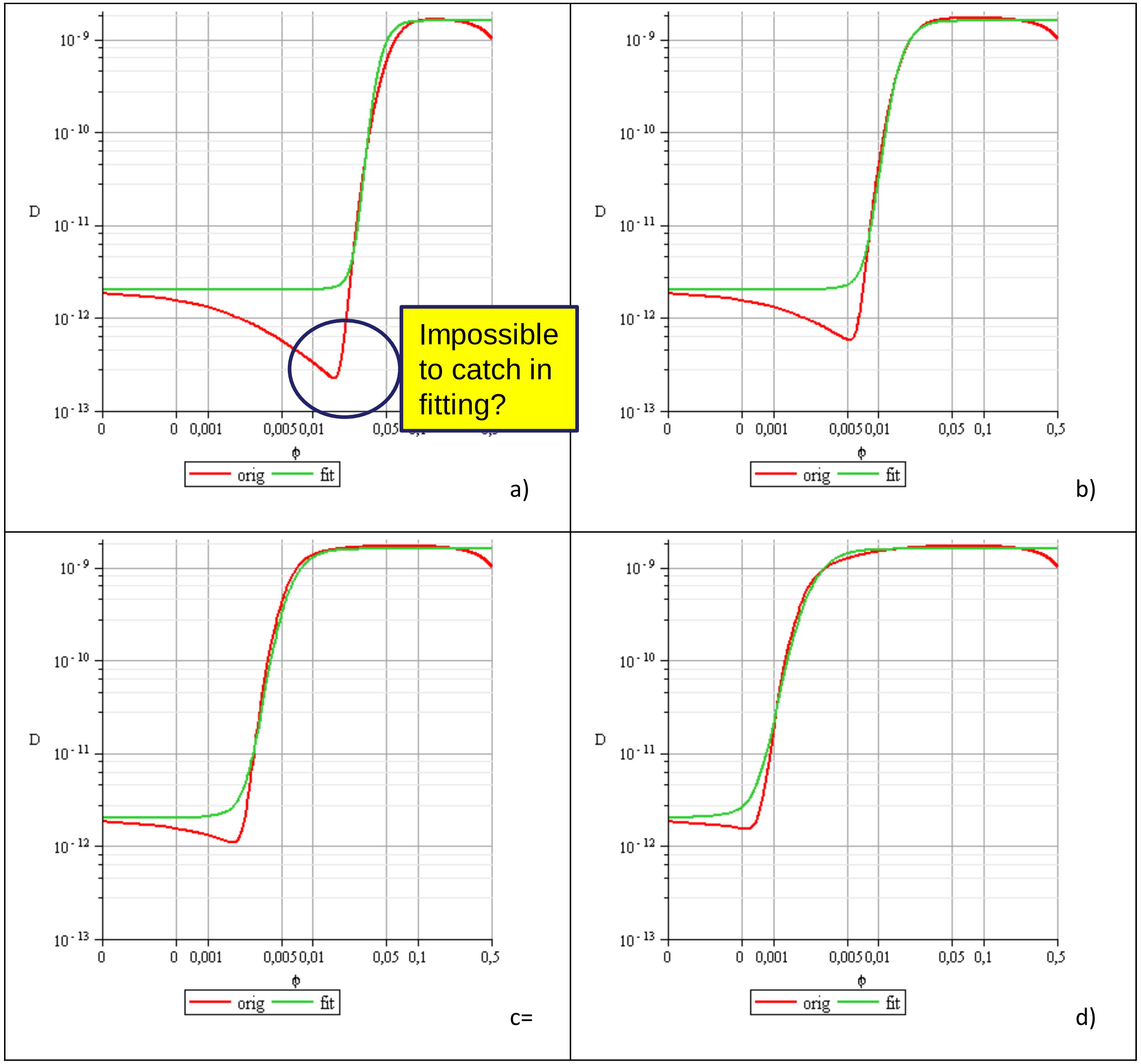
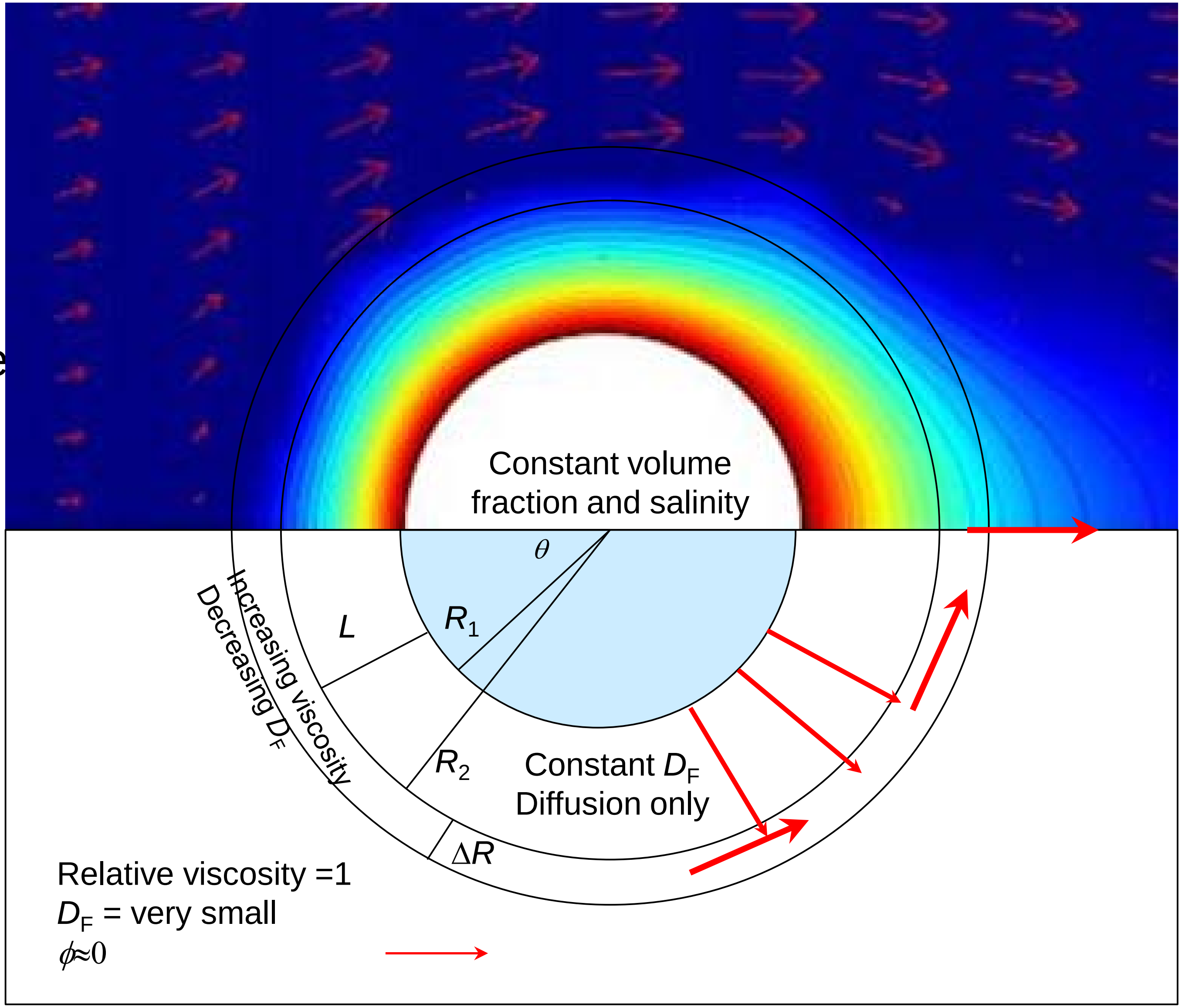


Figure 1. a) 10 mM; b) 1 mM; c) 0.1 mM and d) 0.01 mM

Concept for simple model

- Inner radius *R* (R_1 Fig.)
- Clay ”edge” at $R_2 = R_1 + L$
- After some diffusion math.:
- Enough to know *L* as function groundwater velocity, *v*
- Mass flux per metre at inner radius (the quantity to be estimated by our analysis) will be
- (density, aperture, high diffusivity, volume fraction at boundary)

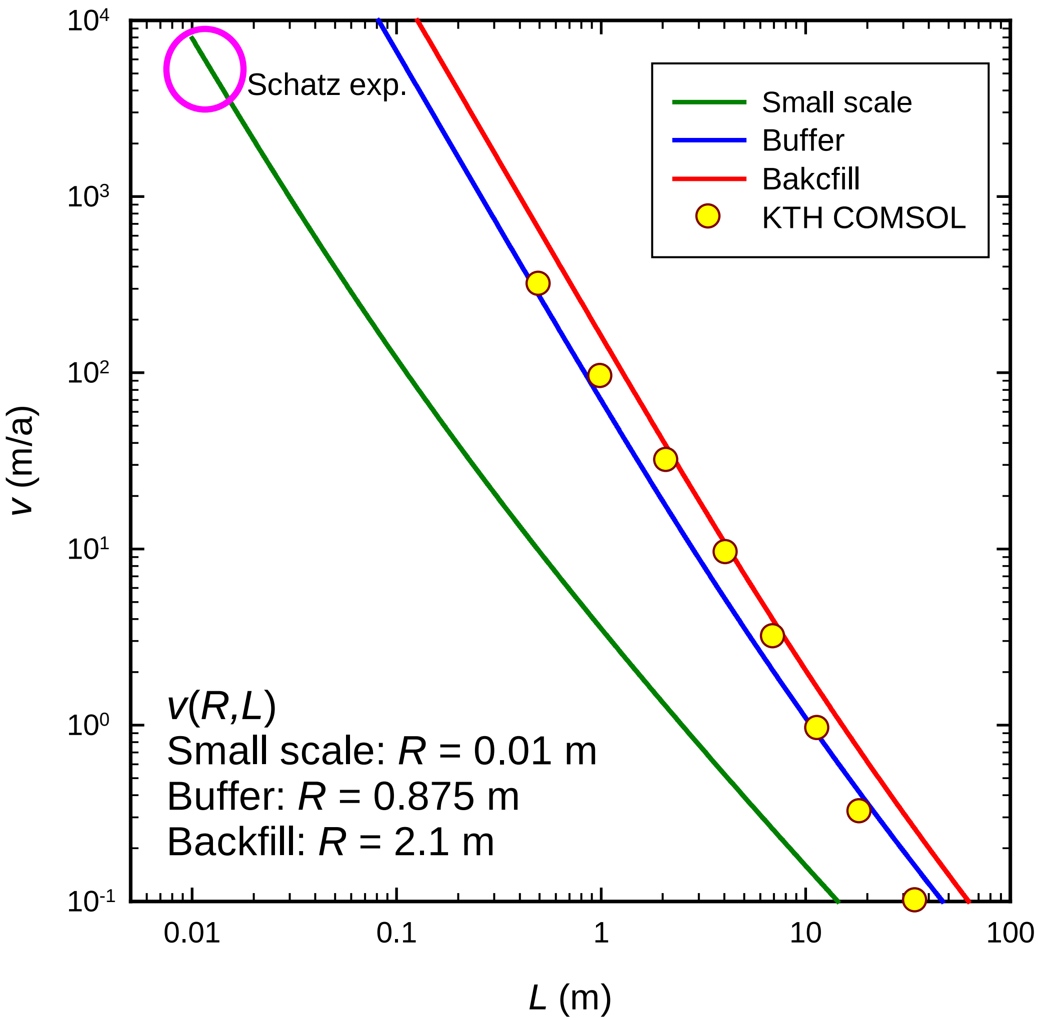
$$q(R_1) = -\rho\delta_S D_F^h \left.\frac{\partial\phi}{\partial r}\right|_{r=R_1} = \frac{D_F^h \rho_S \delta\phi_1}{R_1 \ln\left(\frac{R_1 + L(v)}{R_1}\right)}$$



Correlation between geometry and flow velocity

$$v = A\left(\frac{\phi}{\phi_0}\right)^2 \frac{1}{(R+L)\left[\ln\left(\frac{R+L}{R}\right)\right]^2}$$

- By relatively simple but approximately assumptions it is possible to propose correlation (see Eq.) between the velocity and penetration (extrusion depth), *L*
- Fitting to Neretnieks' model (KTH COMSOL) gives *A* = 76 m^2/a
- Schatz et al. experiments were carried out at high velocity, about 6 000 m/a (see Figure left top corner)
- Therefore, a very simple approximation for penetration depth in the experiments would be 2 cm !
- Note: just knowing *L* enables the estimation of erosion rate!

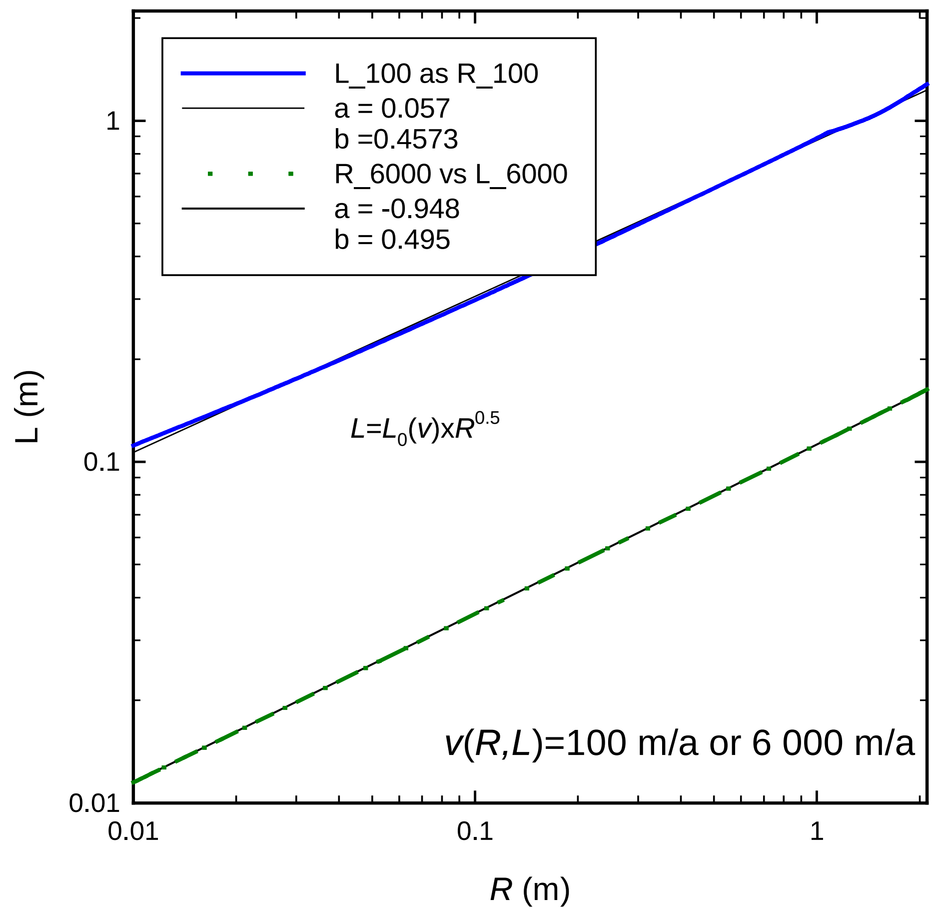


Flux as function of system size

- Total erosion flux increases as **square root of system size,** when extrusion is small (high velocity)

$$L(R,v) = L_0(v)\sqrt{R}$$

$$\begin{aligned} Q(R) &= 2\pi R \times q(R) \\ &= -2\pi R \rho \delta_S D_F^h \left.\frac{\partial \phi}{\partial r}\right|_{r=R} \\ &= \frac{2\pi D_F^h \rho_S \delta \phi_1}{\ln\left(\frac{R+L(R,v)}{R}\right)} \\ &= \frac{2\pi D_F^h \rho_S \delta \phi_1}{\ln\left(1+\frac{L_0(v)}{\sqrt{R}}\right)} \\ &\approx \frac{2\pi D_F^h \rho_S \delta \phi_1}{L_0(v)}\sqrt{R} \end{aligned}$$



Discussion

- If the model is applied at very beginning (diffusivity high over 0.05 volume fractions), the bentonite front may extend as far as hundreds of metres?
- How much there is experimental evidence about the bentonite extrusion into fractures?
- Without any additional internal or external friction term, making the diffusivity much lower, Neretnieks' model predicts extensive extrusion in all conditions?
- Experimental work by Schatz et al done far from the conditions in real repository (spatial scale and velocity)
  - Neretnieks' model by our simplification predicts 0.02 m extrusion and long tail
  - However, experimental observation show almost no tail and larger extension

Conclusions

- At least for VTT, the solution of Neretnieks' original model is hard task
- If analytical formula applied, the modelling is possible at constant salinity
- Simple analysis show that model predicts "erosion" even in saline conditions
- Experimental observations and Neretnieks' model seem to give different, but no so very different results
- In BELBaR
  - Carry out better experiments
  - Develop new models
  - Compare to Neretnieks' model to new approaches

VTT - 70 years of

technology for business and society