Bentonite swelling and erosion. The 2-stage model. Numerical and simplified modelling

Presentation at BELBaR meeting in Meiringen, June 17/18, 2014

Ivars Neretnieks, Luis Moreno, Longcheng Liu

Chemical Engineering and Technology
KTH

Overview of talk

Background

Concept of two-stage model

- Gel/sol viscosity and Bingham properties
- Gel/sol diffusivity

Maths of 2-stage model

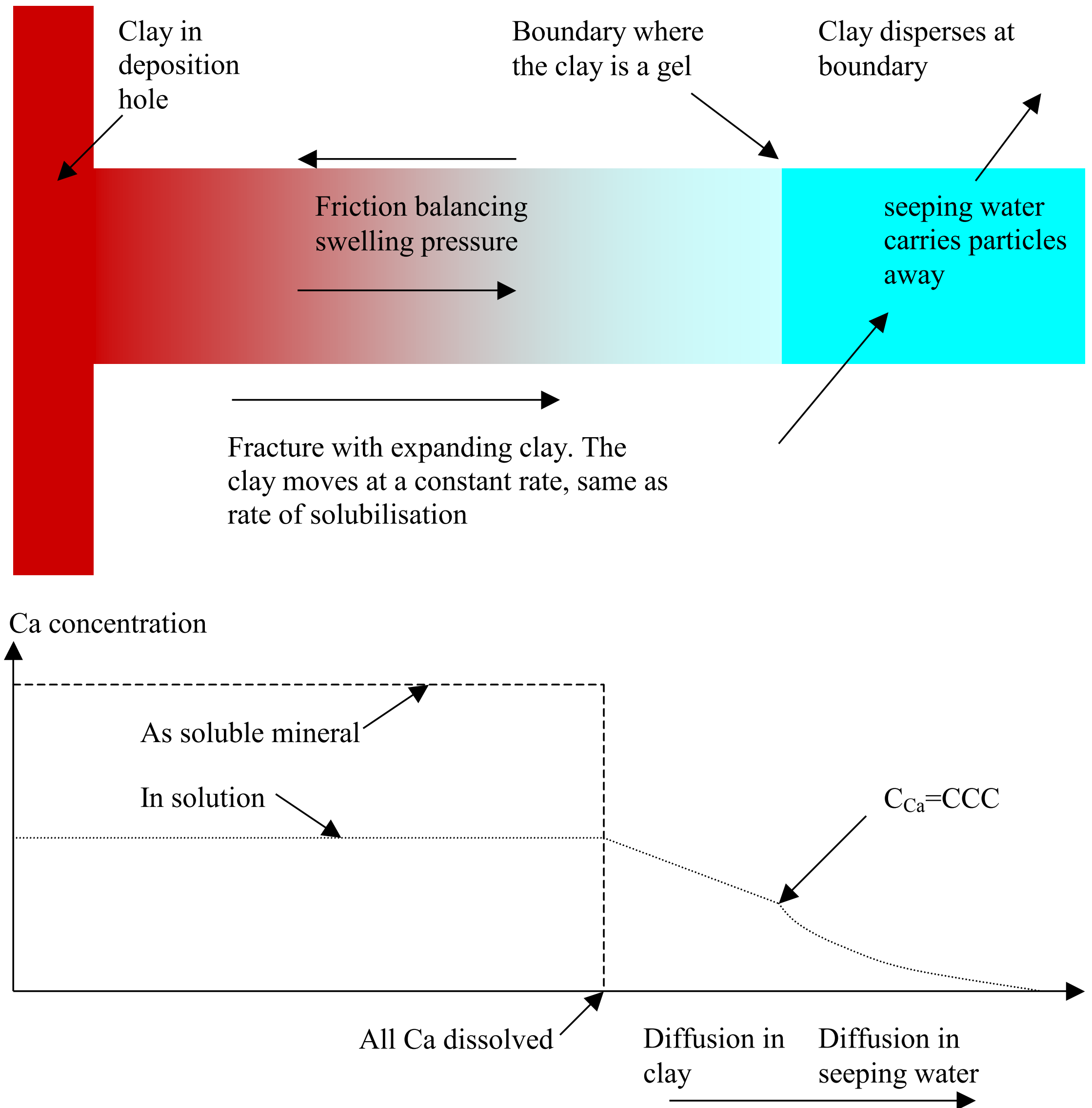
- Numerical solution
- Simplified model

Sample calculations and impact on PA

Background

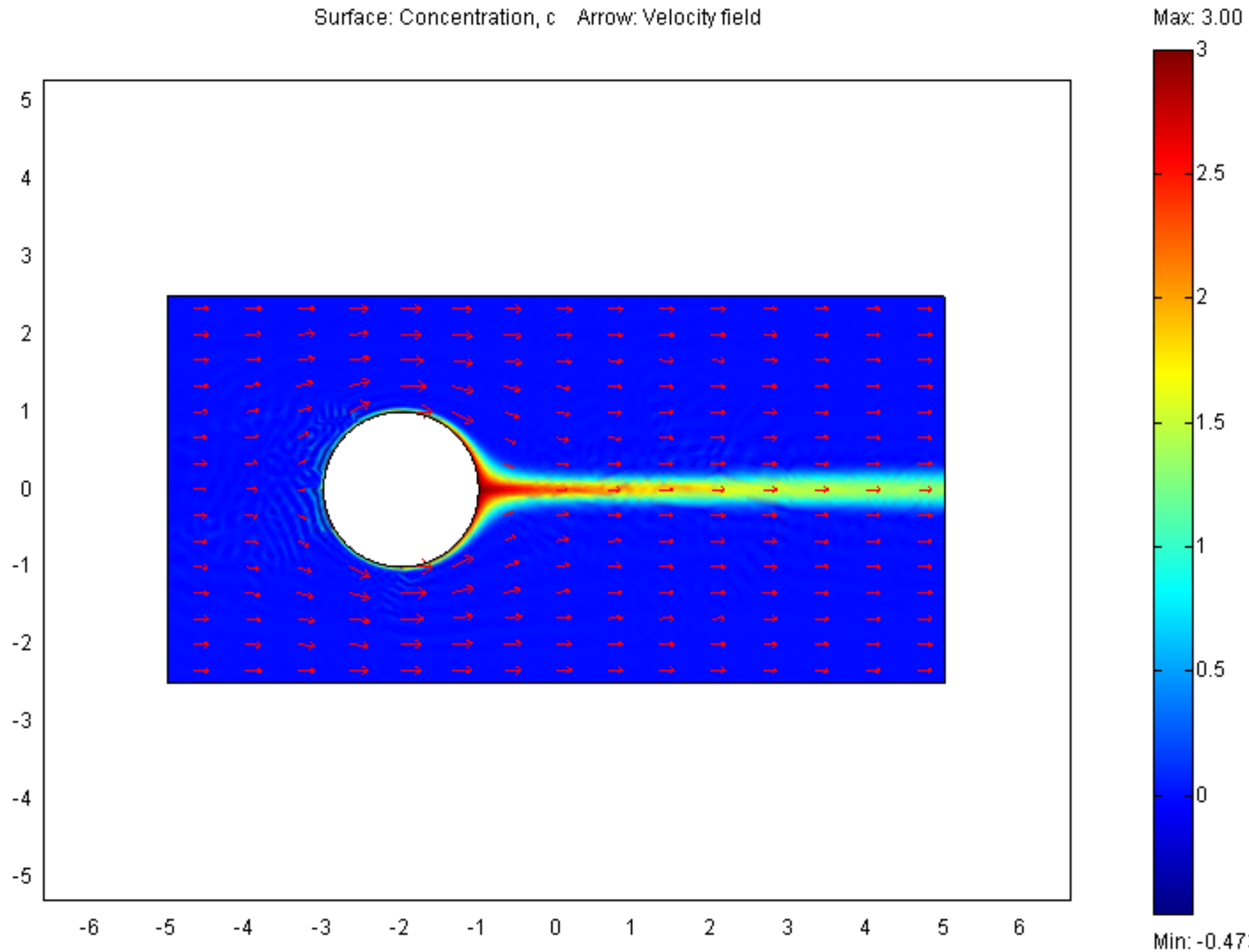
- Previous modeling is based on FEM techniques
- Much to low resolution in the rim zone where the “dramatic” changes occur
- Need to develop new model to resolve rim zone

Transport processes at gel/GW interface



Diffusion to passing GW

Solve the coupled flow and diffusion equations

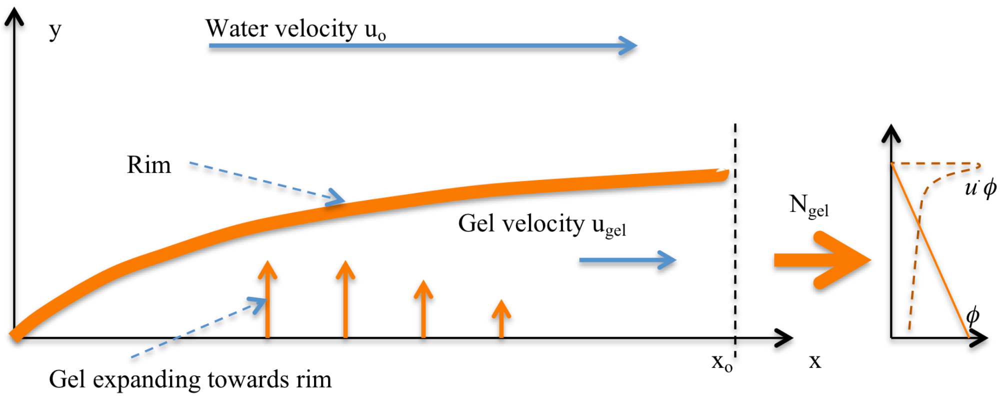


ROYAL INSTITUTE
OF TECHNOLOGY

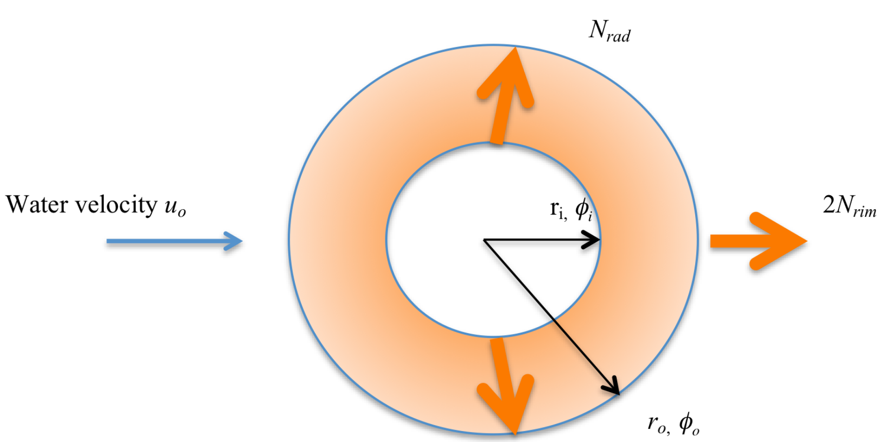
Two-region model

- Inner region 1 metre to more than 100 ds of metres
  - Smectite with volume fraction > *ϕcrit*= 0.004-0.02 (10-50 g/l) does not flow. It can, however, expand by a diffusion-like process
- Sudden jump at *ϕcrit* from no flow to flow
- For PA scales outer, Rim-region- very thin, < 1% of radius of distance to rim
  - At volume fraction < *ϕcrit* it flows with increasing velocity as the viscosity drops

Model expansion and rim separately-then combine models



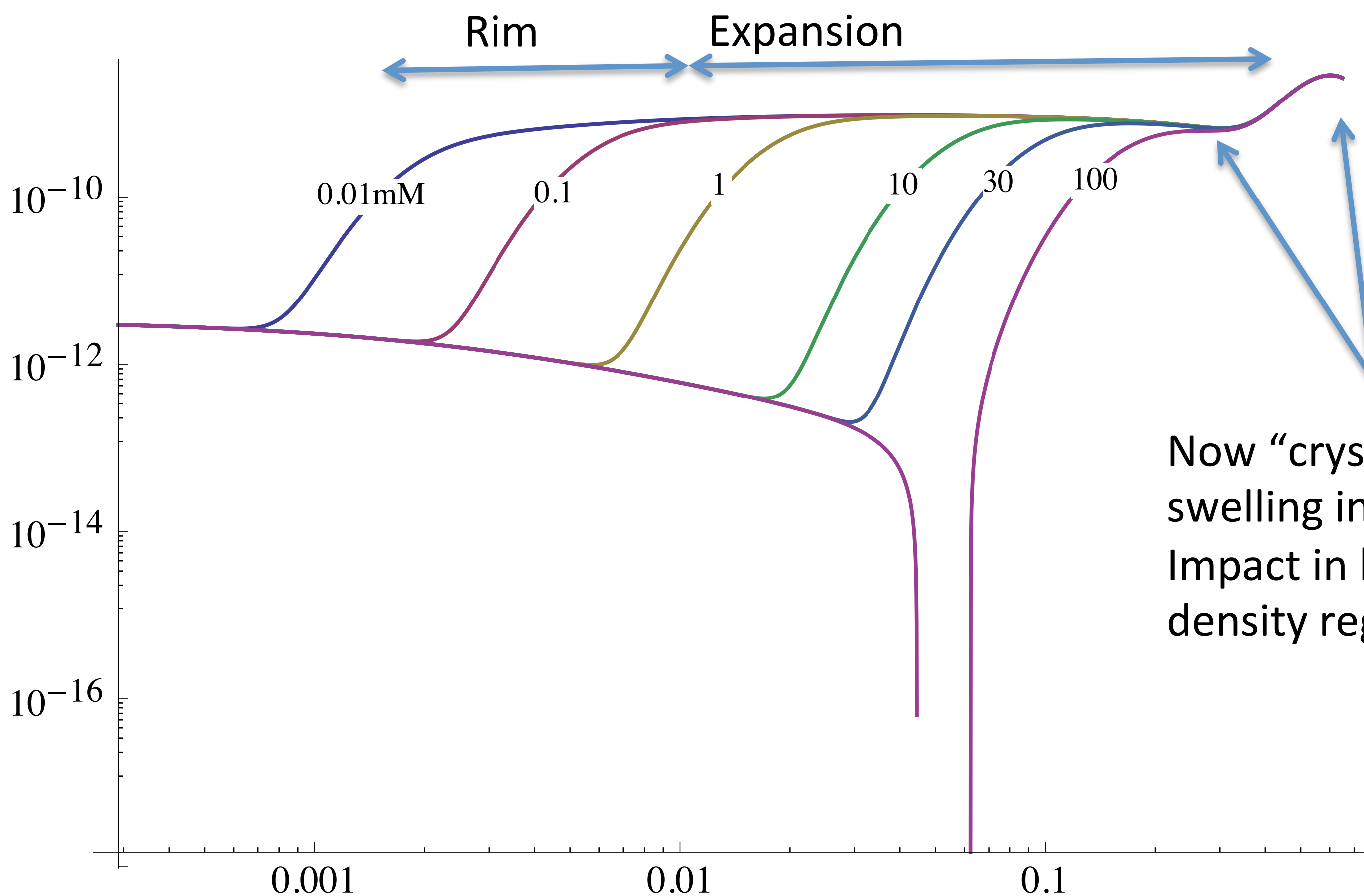
$$N_{rim} \propto f(\phi_i)\delta_{frac}\sqrt{2\pi r_0}$$



Loss from deposition hole is mass that goes into fracture N_{loss}-

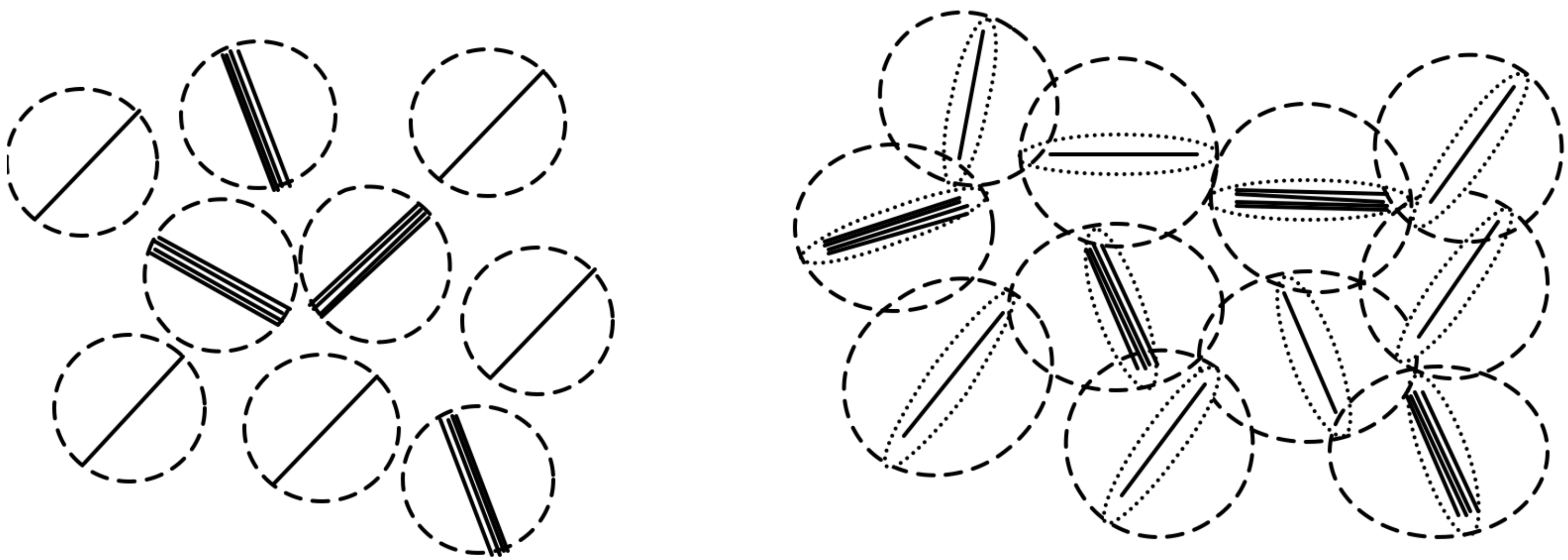
Once steady state is reached expansion ceases and N_{loss}=N_{rim}-

Diffusion function of gel/sol



Now “crystalline” swelling included. Impact in high density region

Co-volume concept



Thin diffuse double layer, co-volumes do not overlap

Large diffuse double layer, co-volumes overlap

Figure 5.1 Illustration of co-volume with and without impact of diffuse layer for a given ϕ. The extent of the diffuse layer is shown as dotted oval in the right figure.

Model of gel/sol viscosity

$$\frac{\eta}{\eta_w} = 1 + 1.022\varphi_{cov}^{\kappa} + 1.358(\varphi_{cov}^{\kappa})^3$$

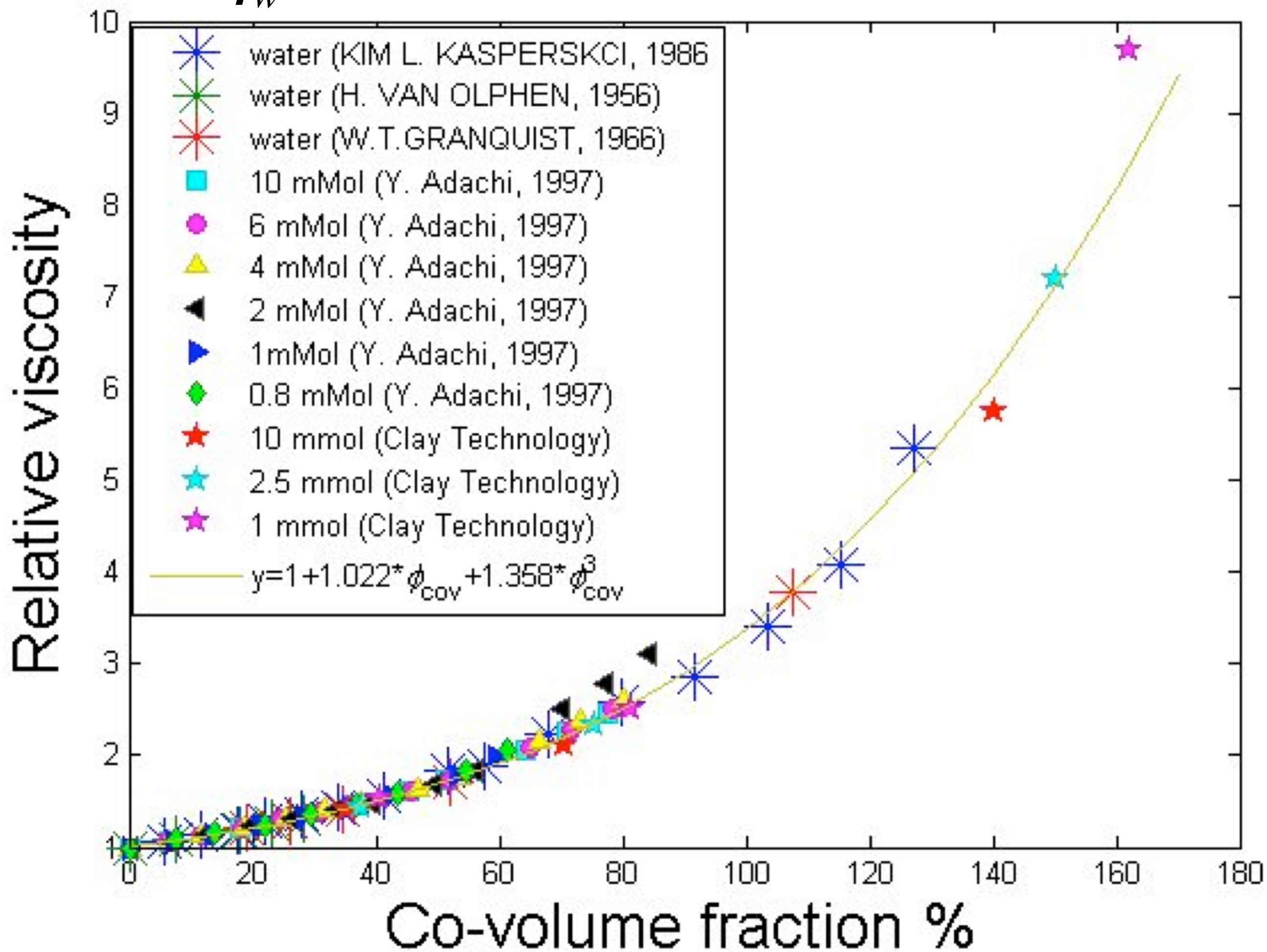


Figure 5.5 Relative viscosity as a function of co-volume fraction from different

Basic equations for rim loss

$$D_{rel}(\phi)\frac{\partial^2\phi}{\partial y^2}+\frac{dD_{rel}(\phi)}{d\phi}\left(\frac{\partial\phi}{\partial y}\right)^2=\frac{u_o}{D_o\eta_r(\phi)}\frac{\partial\phi}{\partial x}$$

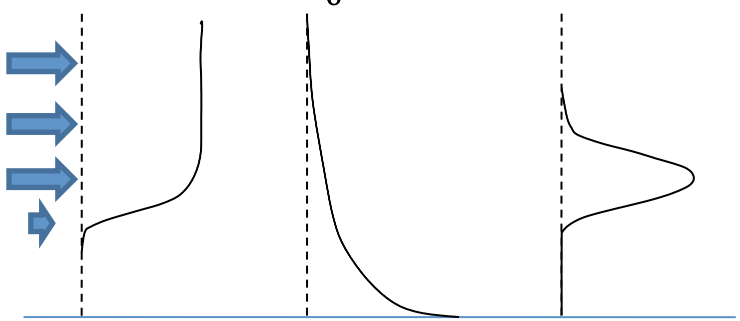
PDE

$$z=\frac{y}{2\sqrt{D_o x/u_o}}$$

$$\eta_r(\phi)D_r(\phi)\frac{d^2\phi}{dz^2}+\eta_r(\phi)\frac{dD_r(\phi)}{d\phi}\left(\frac{d\phi}{dz}\right)^2=-2z\frac{d\phi}{dz}$$

ODE to be solved w arbitrary accuracy

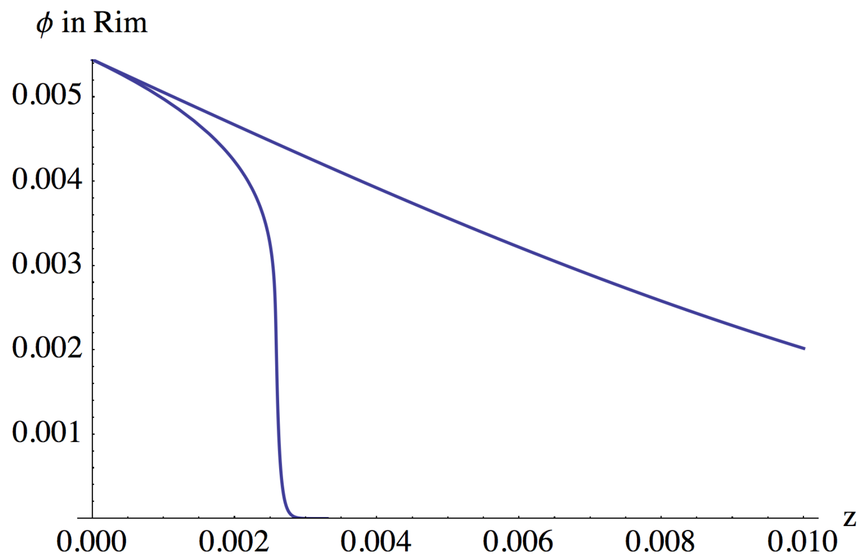
$$N_{rim}=\delta_{frac}\int_0^\infty u(y)\phi(y)dy=\delta_{frac}u_o\int_0^\infty\frac{\phi(y)}{\eta_{rel}(\phi(y))}dy$$



$$N_{rim}=N_{rim}^{DL}\delta_{fr}2\sqrt{D_o x u_o}$$

Only depends on ion
conc. surface charge
density and particle size

Example: c=0.1 mM



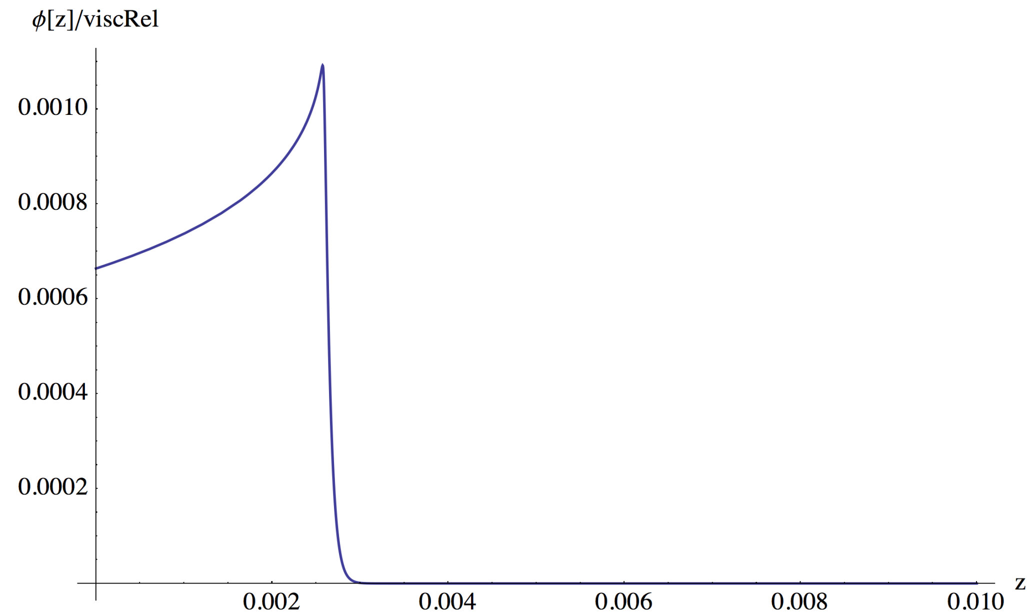


Figure 7.6. Relative measure of the flux ϕu *in the rim zone, u=10*$^{-5}$ *m/s and c=0.1 mM. Left figure is for* $\phi_{Cov} = 1.6$.

Figure 7.5 concentration profile in the rim zone, $\phi_{Cov} = 1.6$*, u=10*$^{-5}$ *m/s and c=0.1 mM monovalent ions. Right hand curve is for constant D and viscosity.*

$$z = \frac{y}{2\sqrt{D_o x/u_o}}$$

Instationary phase of gel expansion in region r_i to r_R

$$\frac{\partial\ \phi}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(Dr\,\frac{\partial \phi}{\partial r}\right) - \frac{dr_R}{dt}\frac{\phi}{r_R - r_i}\left(1 + \frac{r - r_i}{r}\right)$$

$$\frac{dr_R}{dt} = \frac{N_{in} - 2N_{rim}(r_R)}{\varrho_s \delta_{fr} \pi 2\phi_{mean}}\frac{dr_R}{dt} - \frac{d\phi_{mean}}{dt}\frac{(r_R^2 - r_i^2)}{r_R 2\phi_{mean}}$$

$$N_{rim} = N_{rim}^{DL}\delta_{fr} 2\sqrt{\ D_o x u_o}$$

Combine rim with expansion of gel

- Let the gel expand and account all the time for the loss at the rim
- Numerical solution of the PDE in region

ri –rR(t). *rR(t)* constantly expands

- Loss at rim as BC
- N_{rim} solved with arbitrarily high resolution

Two solution techniques for expanding grid

- Numeric solution of the PDE in expanding grid w. modified Crank-Nicolson technique. Sometimes numerical difficulties
- Analytical solution based on PSS assumption useful when *D* fairly constant except at rim. Analytical- very simple expressions
- Surprisingly small differences

Example

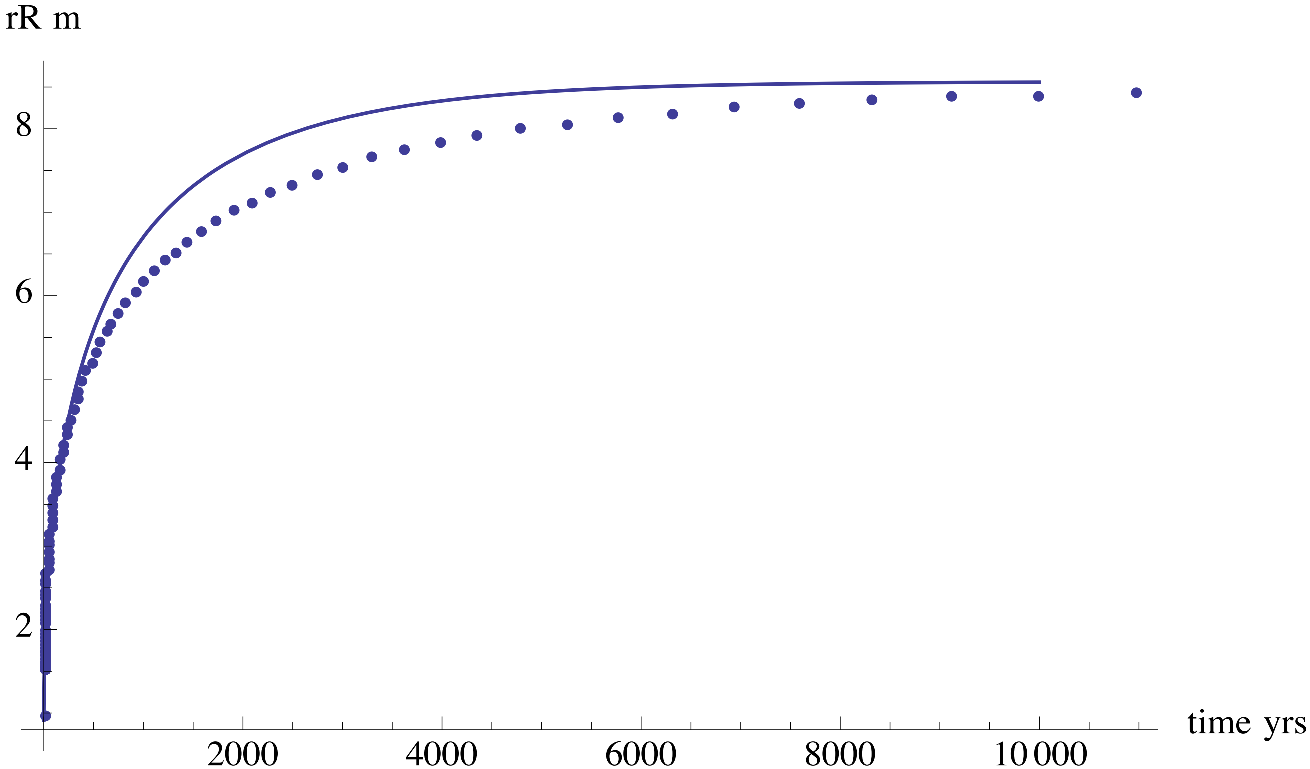


Figure xx. Expansion of the rim for c=0.1 mM and $u_o=10^{-5}$ *m/s,* $\phi_i = 0.5, = 0.32\times10^{-9}$ m^2/s
d_p*=200 nm. Dots are numeric solution and line is the PSS solution.*

0.1 mm aperture, 10^{-5} m/s (315 m/yr)

c mM	*r_R at SS m*	*N_{SS} g/year*	*Mass in fracture kg at SS*
0.1	14.4	4.7	10.8
1	32.1	3.1	47.0
10	29.1	3.0	63.9

For lower flowrates rR at SS increases enormously, as does tome to approach SS. Loss is dominated by intrusion into fracture, not by erosion at Rim

Impact on PA

- Smectite loss from deposition hole at lower flowrates dominated by intrusion far into fracture
- Only extremely high flowrates may cause loss by erosion to be considered
- Smectite will invade even the finest fractures and generate a strong diffusion barrier to decrease solute transport to and from the canister

Processes not modeled

- Loss by gravity pulling off aggregates
  - Observed by Schatz and Neretnieks
- Fate of detritus material
  - The fine sand may clog the variable aperture fractures
  - Hinder further expansion of smectite into fracture

What next

- Prepare report on the model development
- Use the model(s) to analyze available experiments
- Ponder the gravity effects

Thank you for your attention