# Smectite erosion model- testing model simplification

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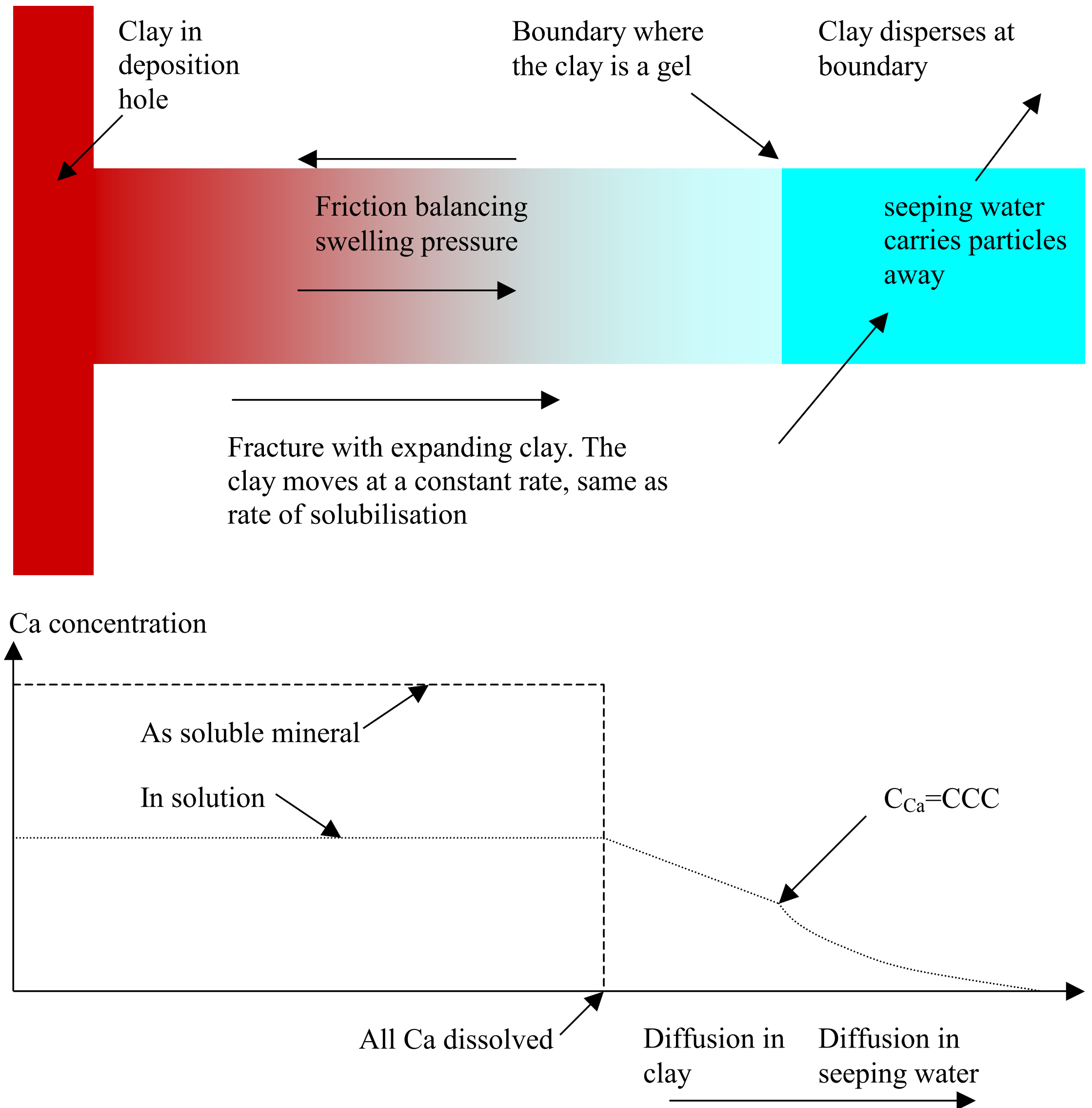
KTH Chemical Science and Engineering

# Erosion of smectite

- Fresh water solubilizes smectite
- High flowrates around a deposition hole

# Transport processes at gel/GW interface

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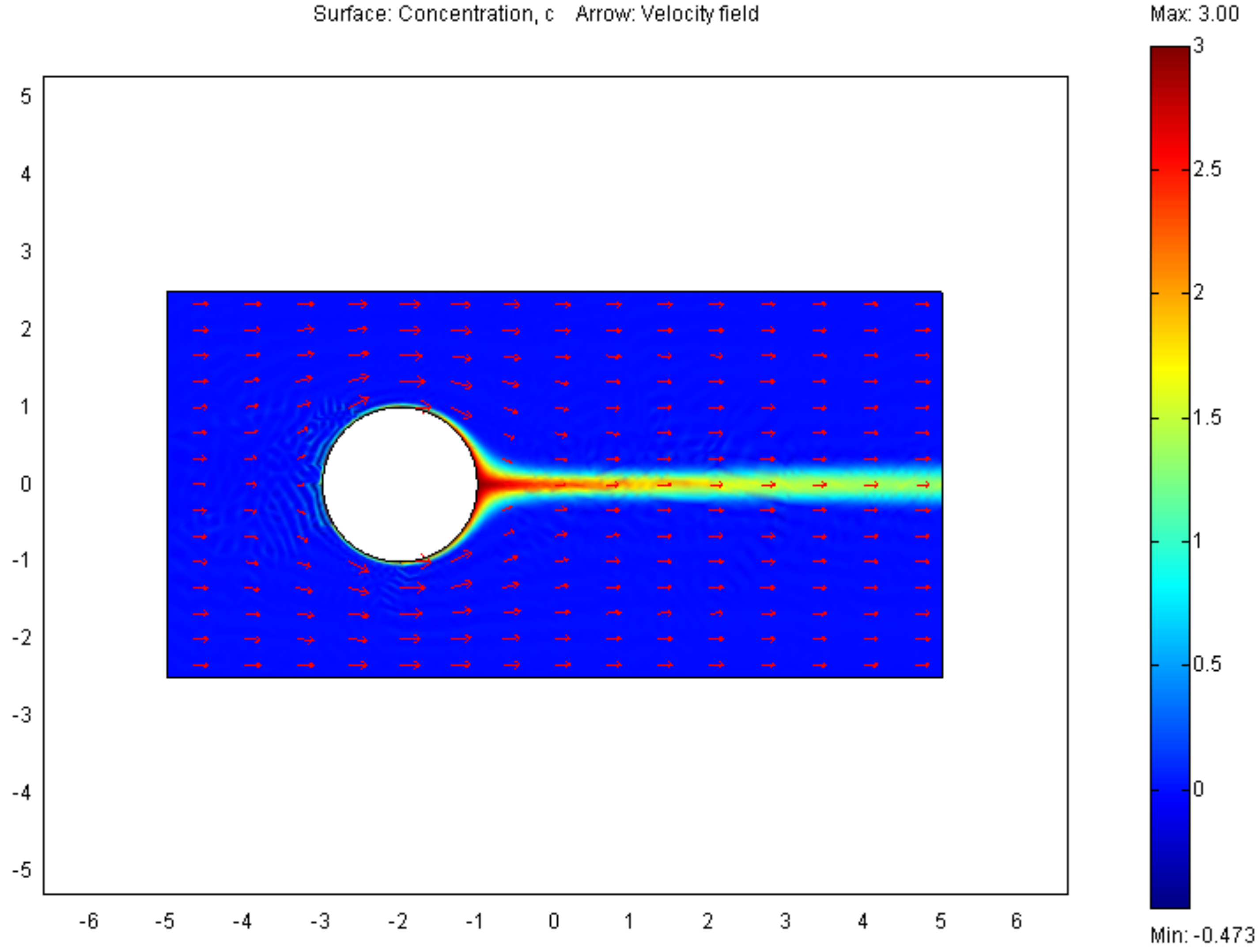
# Diffusion to passing GW

# Solve the coupled flow and diffusion equations

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# Main competing mechanisms

- Smectite swells by a diffusion-like process into the seeping water
- Gel/sol viscosity increases greatly with volume fraction

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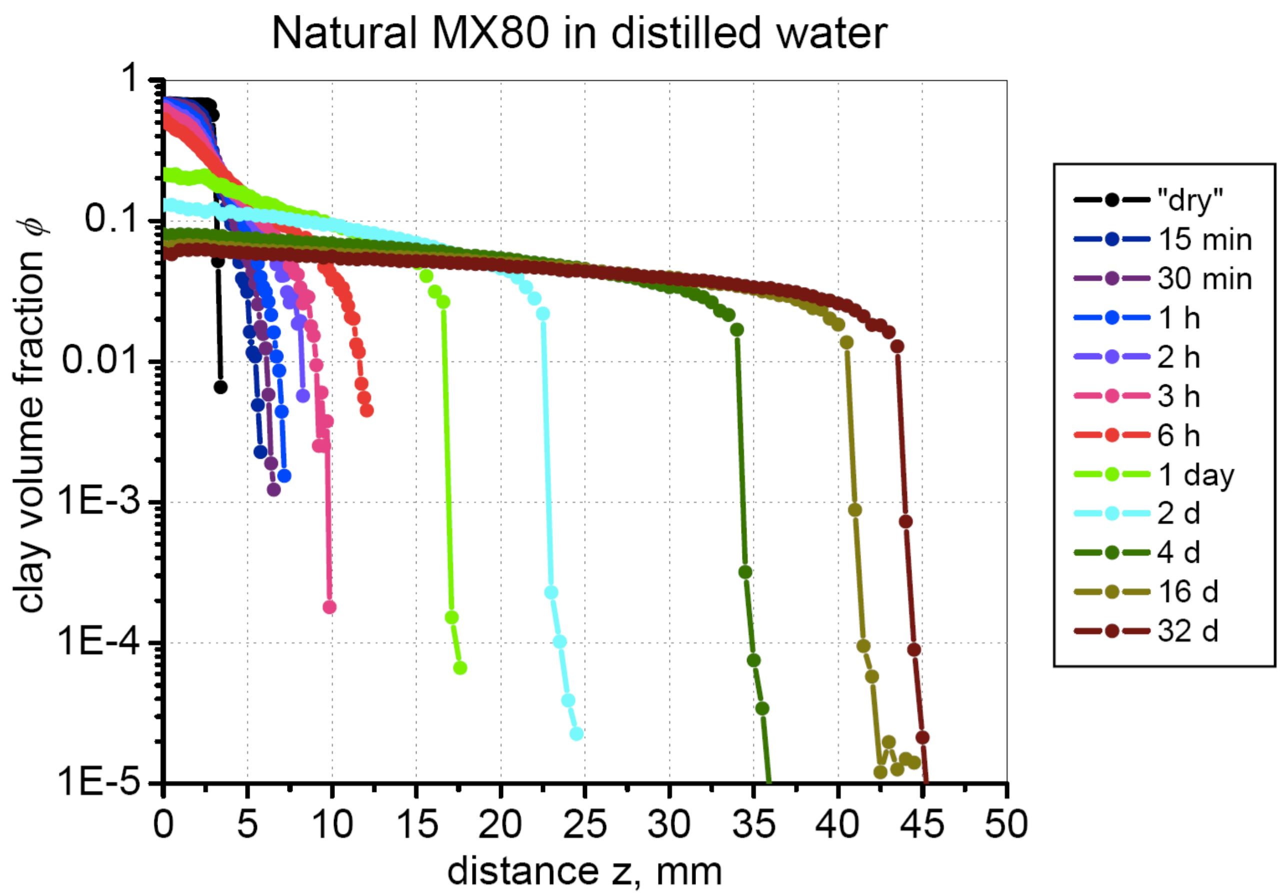
# Diffusion profiles- measured

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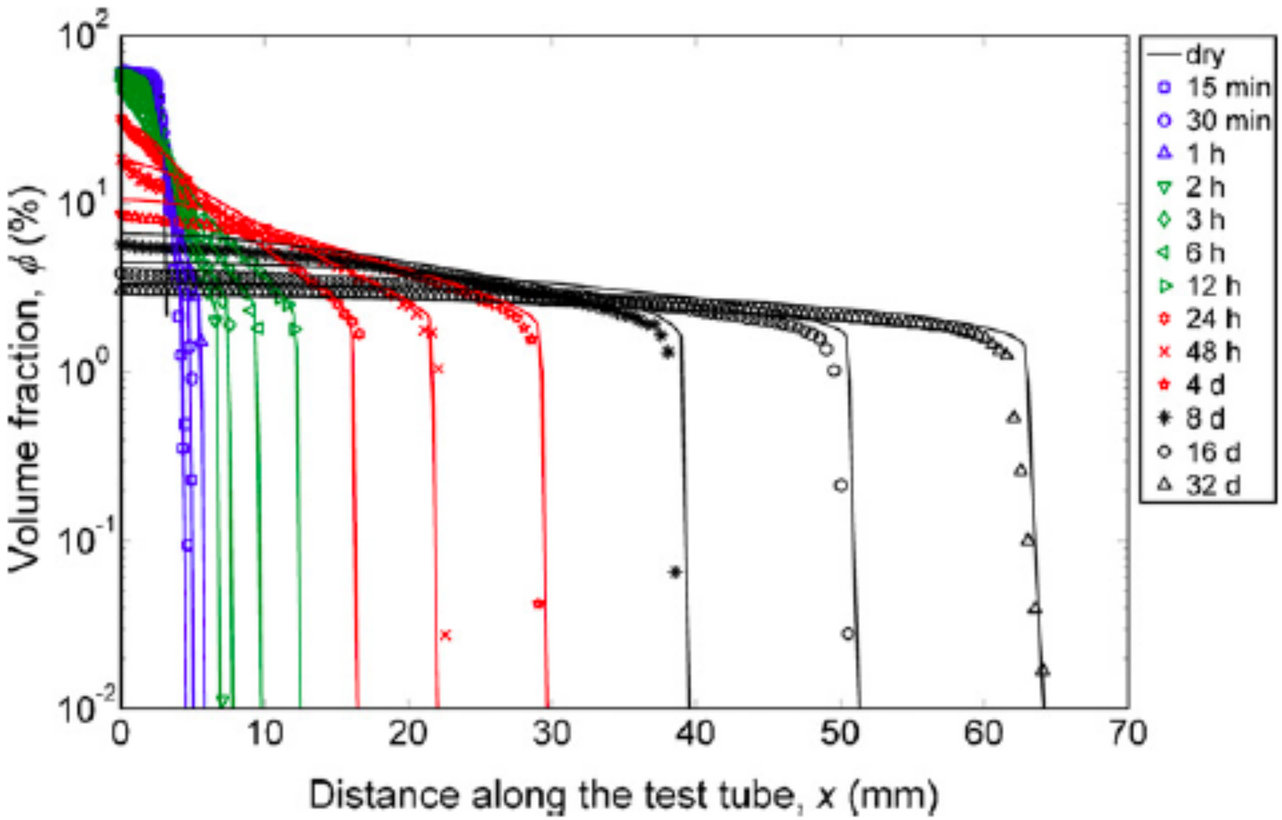
# Model prediction of experiment

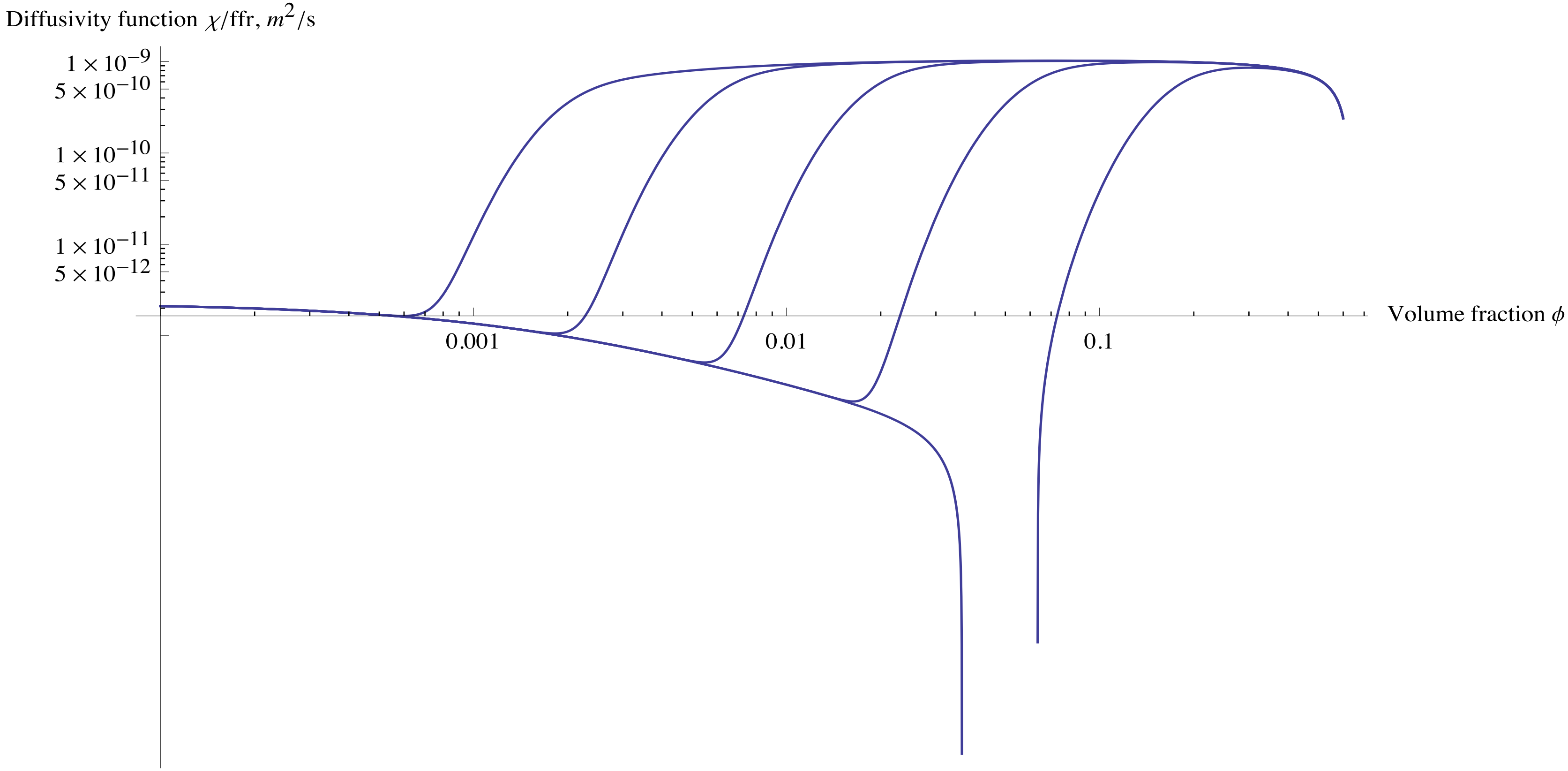



Balance of swelling force and friction force of particle in water,
Liu L.

**Fig. 7.** Measured versus predicted expansion of WyNa in 0.5 mM $CaCl_2$ solution in logarithmic scale. The KC-like equation is used and the particle thickness is 1.5 nm.

Colloids and Surfaces A: Physicochem. Eng. Aspects 358 (2010) 68–78

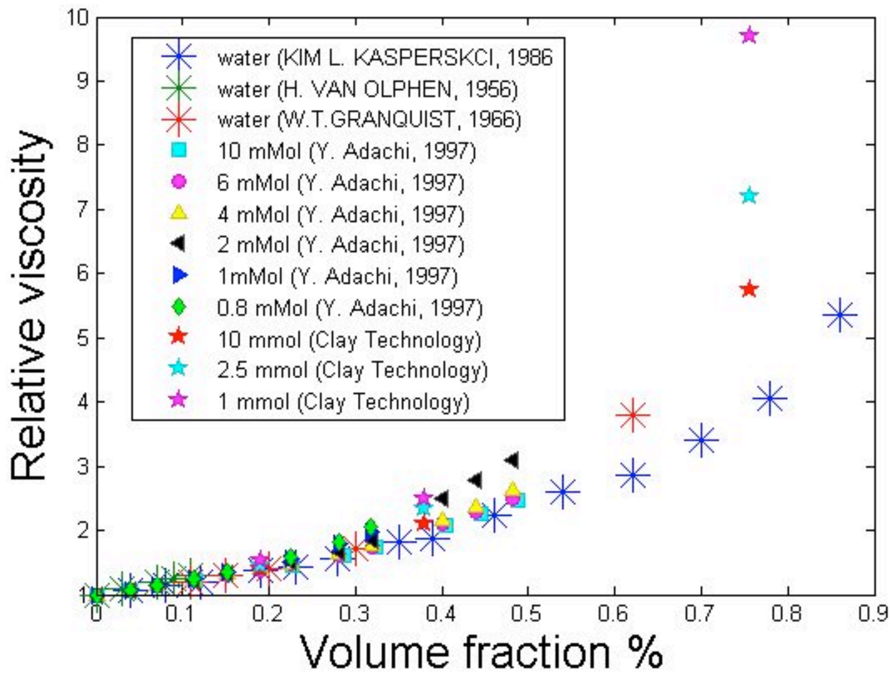
# Diffusion function



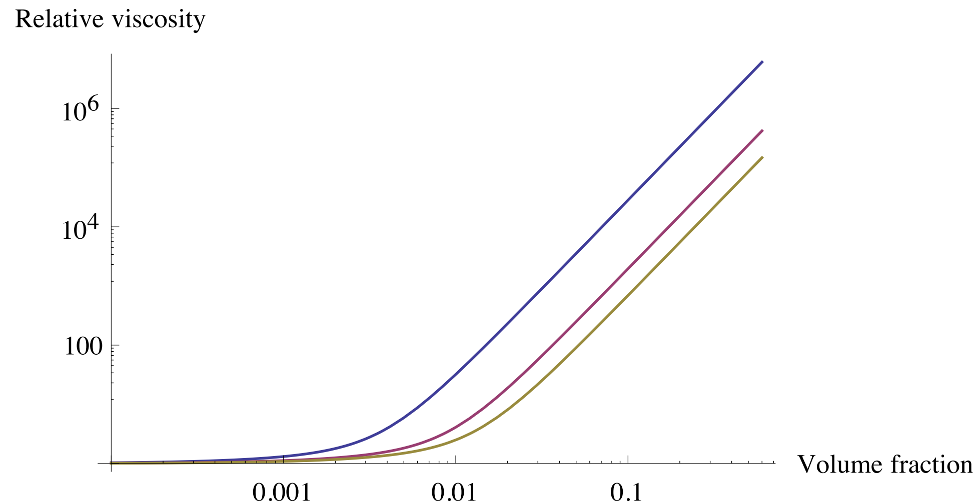

*The curves from left to right are for 0.01, 0.1, 1, 10, and 100 mM ion for z=1, $\delta_p$ =$10^{-9}$ m and $\sigma_0$=-0.131 C/$m^2$*

Liu et al. Langmuir 2009, 25, 679-687 679

# Gel/sol viscosity



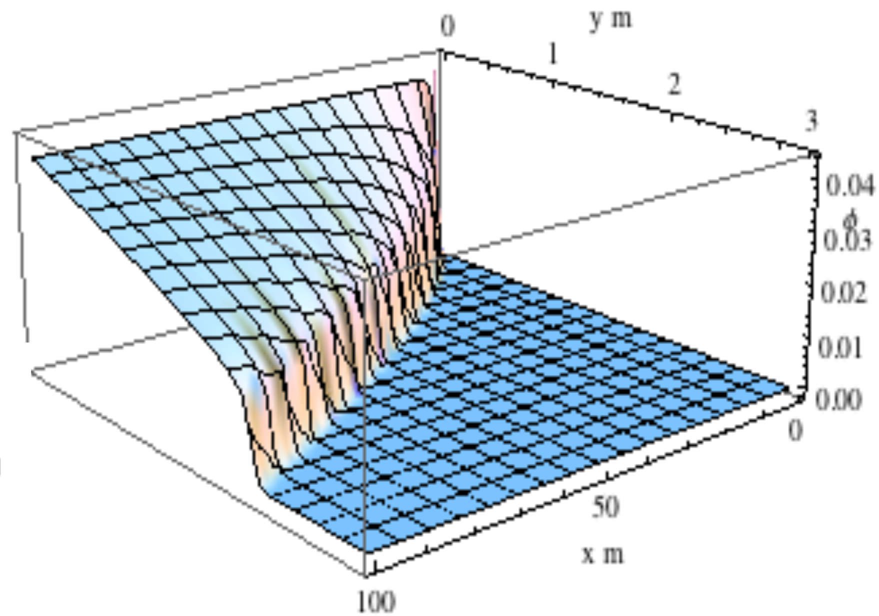

Liu L. Physics and Chemistry of the Earth 36 (2011) 1792–1798



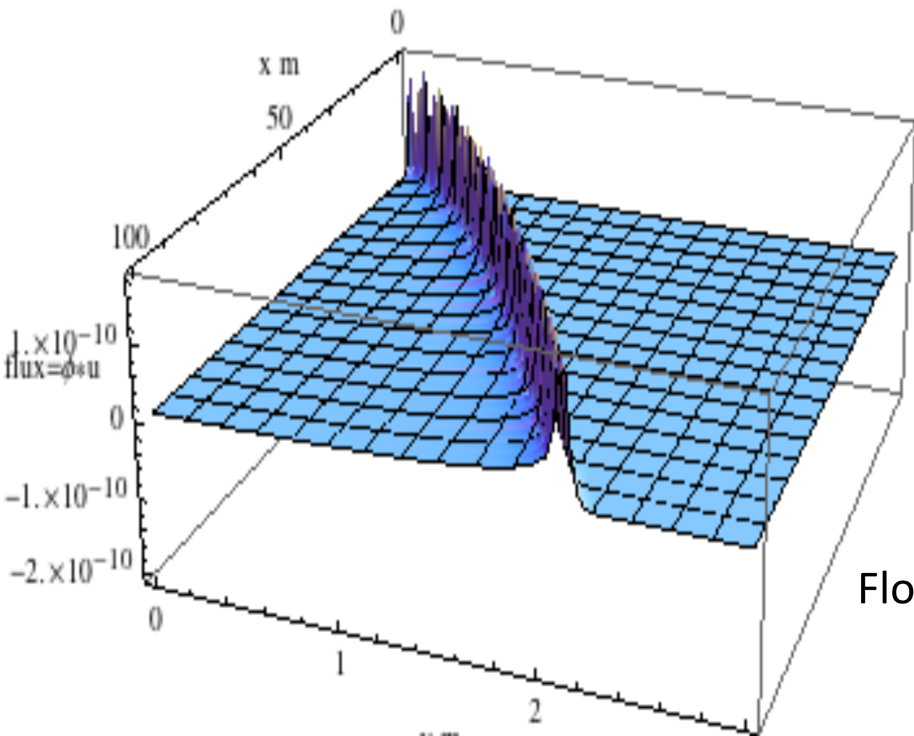
# Equations, sample simulations

$$\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x} D(\phi) \frac{\partial \phi}{\partial x} + \frac{\partial}{\partial y} D(\phi) \frac{\partial \phi}{\partial y} - u_x \frac{\partial \phi}{\partial x} - u_y \frac{\partial \phi}{\partial y}$$

$$u_x = -T_o \frac{\delta_{frac}}{\rho g \eta(\phi)} \frac{dP}{dx}$$

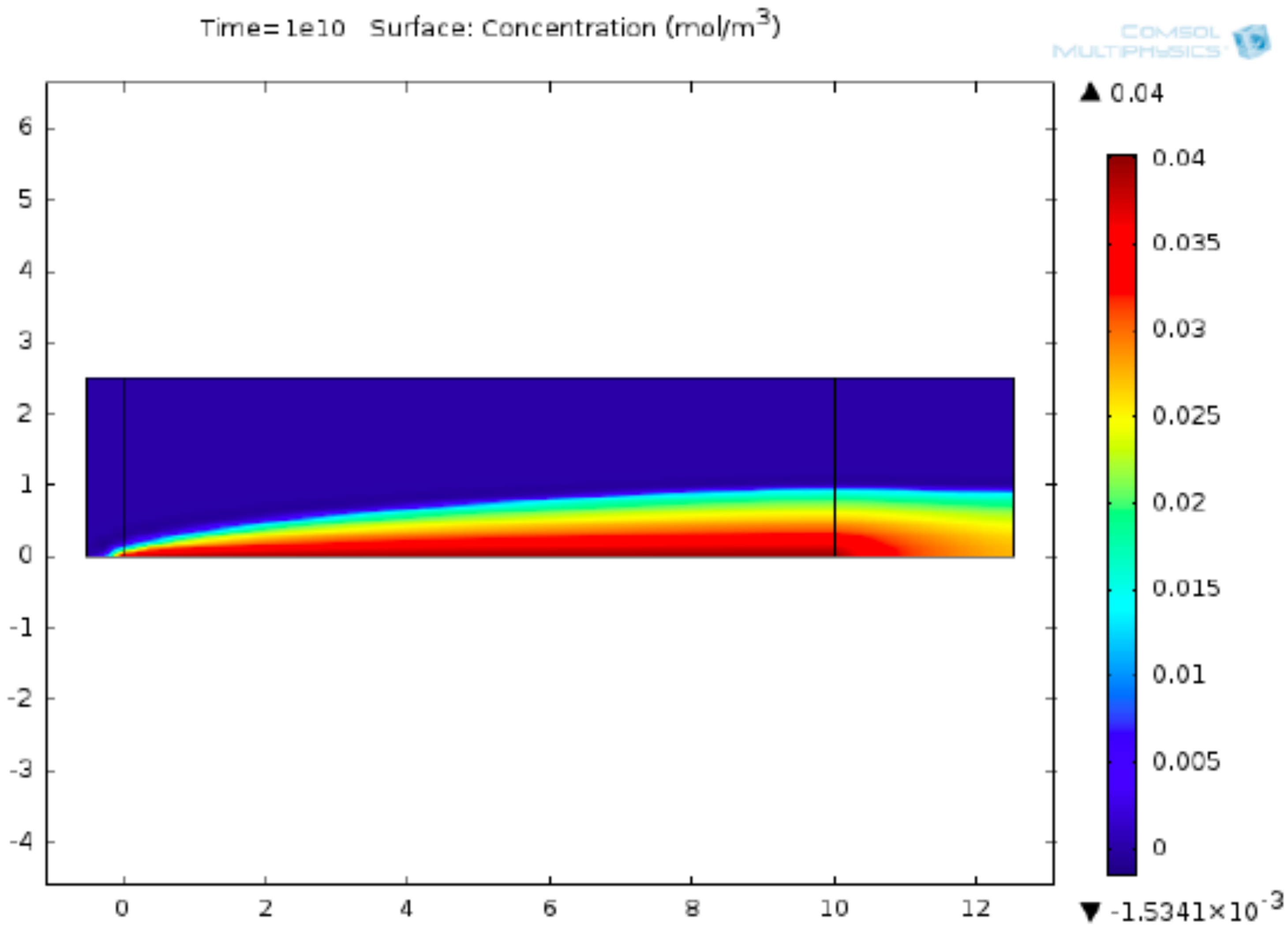



Concentration (t1,x,y)

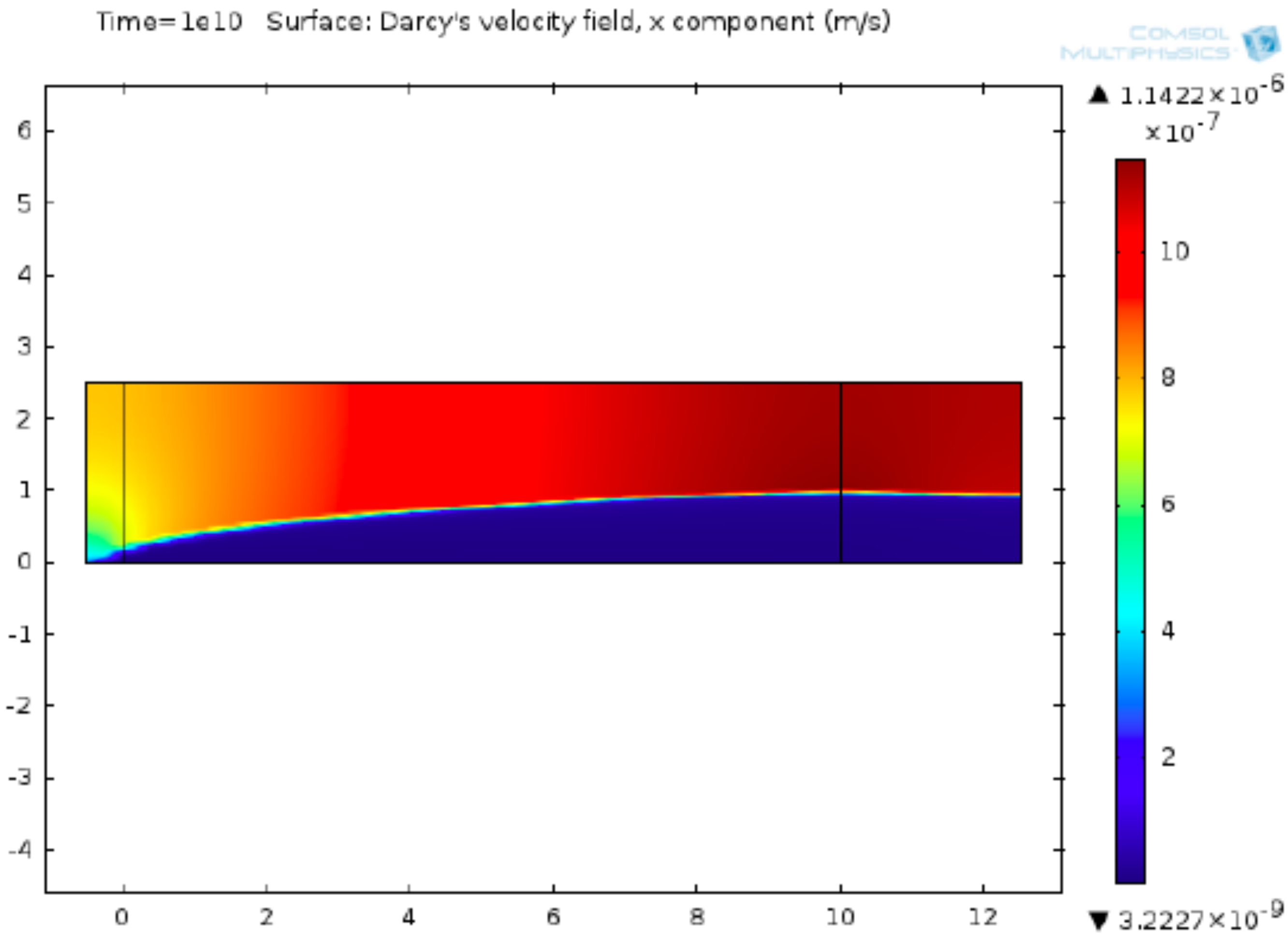



Flowrate(t1,x,y

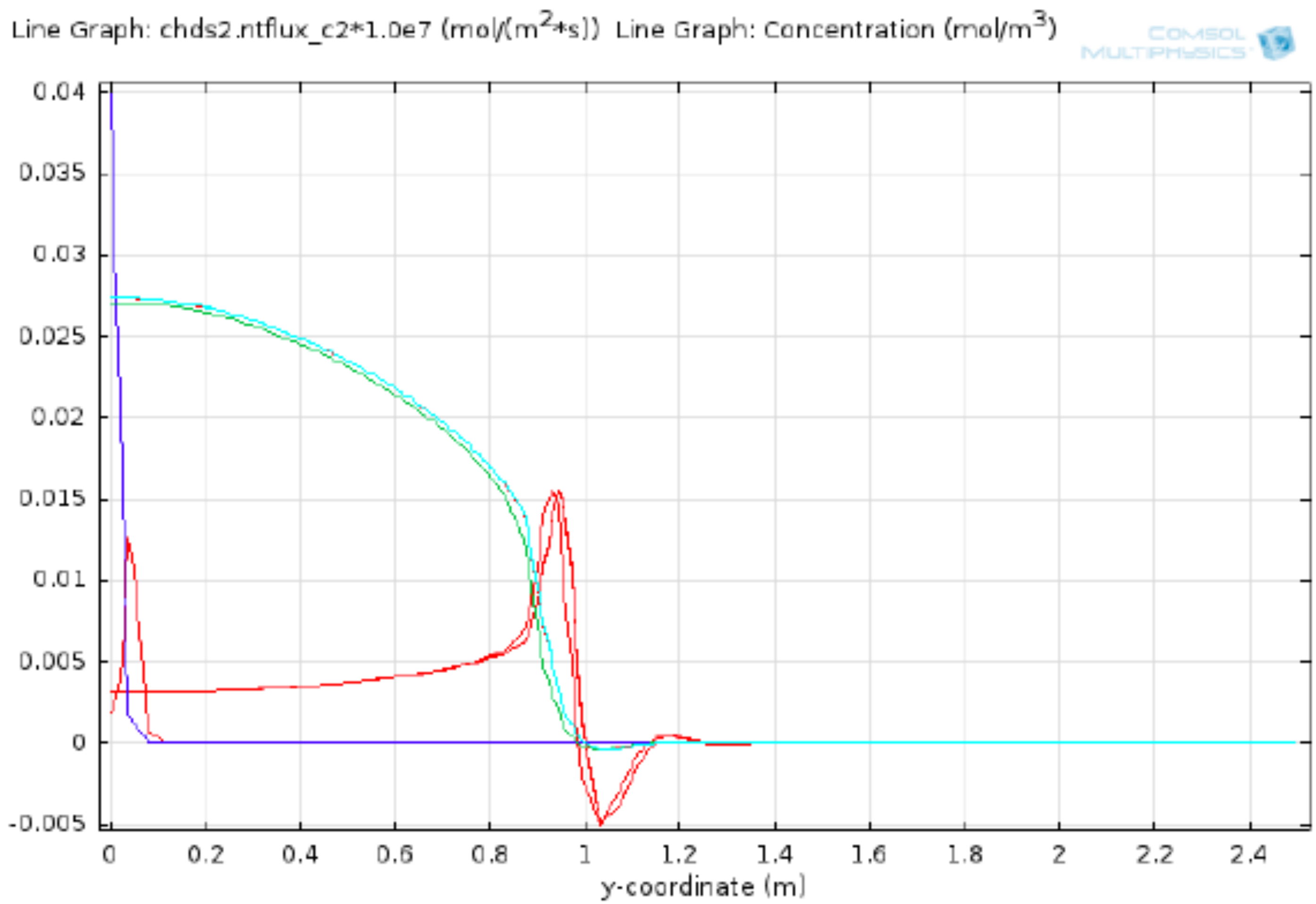
# Concentration profile



# Flow velocity



# Concentration and Smectite flowrate



# Concerns

- We and others have experienced difficulties of solving the eqs in several important cases
- Modern tools e.g. Comsol Multiphysics® and Mathematica® are not robust for the very sharp fronts
- Results may be erroneous by unknown quantity even when results are obtained

# Everything happens in a thin rim- Causes numerical difficulties

- Gain insights into when different mechanisms are important
  - Flow
  - Diffusion
  - viscosity
- Improve numerical techniques
  - Finer grids in Finite element/difference methods
  - Adaptive grids?
- Simplify equations – next slide

# Simplify equations for linear flow

$$\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x} D(\phi) \frac{\partial \phi}{\partial x} + \frac{\partial}{\partial y} D(\phi) \frac{\partial \phi}{\partial y} - u_x \frac{\partial \phi}{\partial x} - u_y \frac{\partial \phi}{\partial y}$$

Often we are interested in Steady State. Omit term

Gradient in flow direction (x) << than in perpendicular direction

Smaller than in flow direction, but….

# After some manipulation transformation

$$f1(\phi)\frac{d^2\phi}{dz^2} + f2(\phi)(\frac{d\phi}{dz})^2 = -2z\frac{d\phi}{dz} \qquad z = \frac{y}{\sqrt{4x}}$$

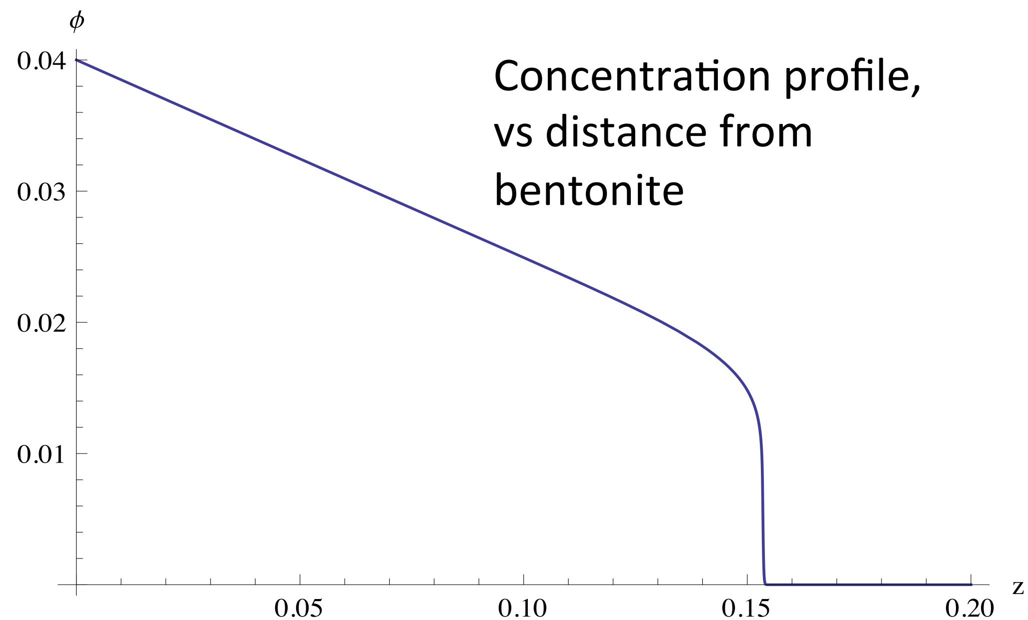
$$f1(\phi) = \frac{\eta(\phi)D(\phi)}{u_o} \qquad f2(\phi) = \frac{\eta(\phi)}{u_o}\frac{dD(\phi)}{d\phi}$$

$$z = 0 \quad \phi = \phi_o \qquad\qquad z \rightarrow \infty \quad \phi = 0$$

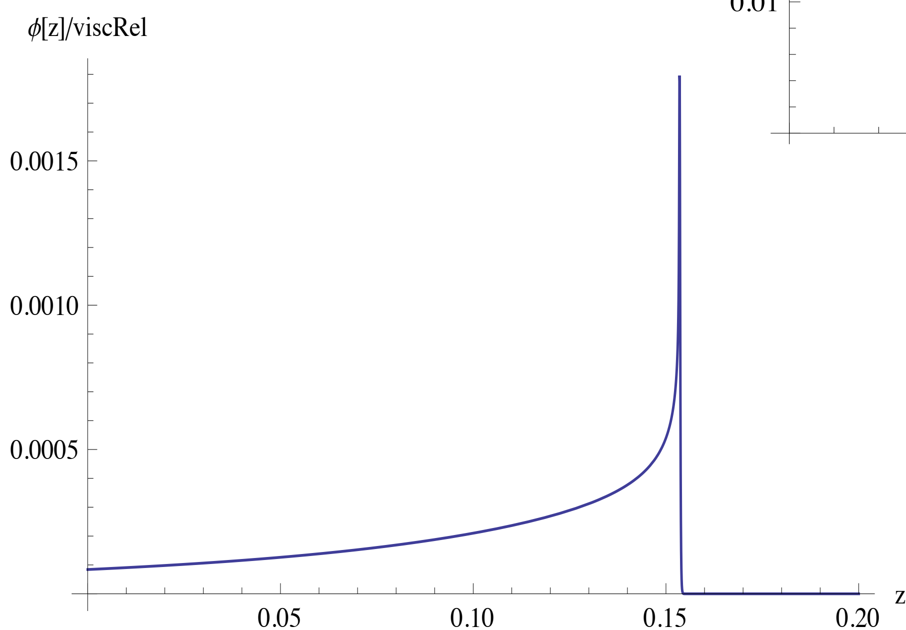
One ODE results as a boundary value problem !

# Some results for the ODE

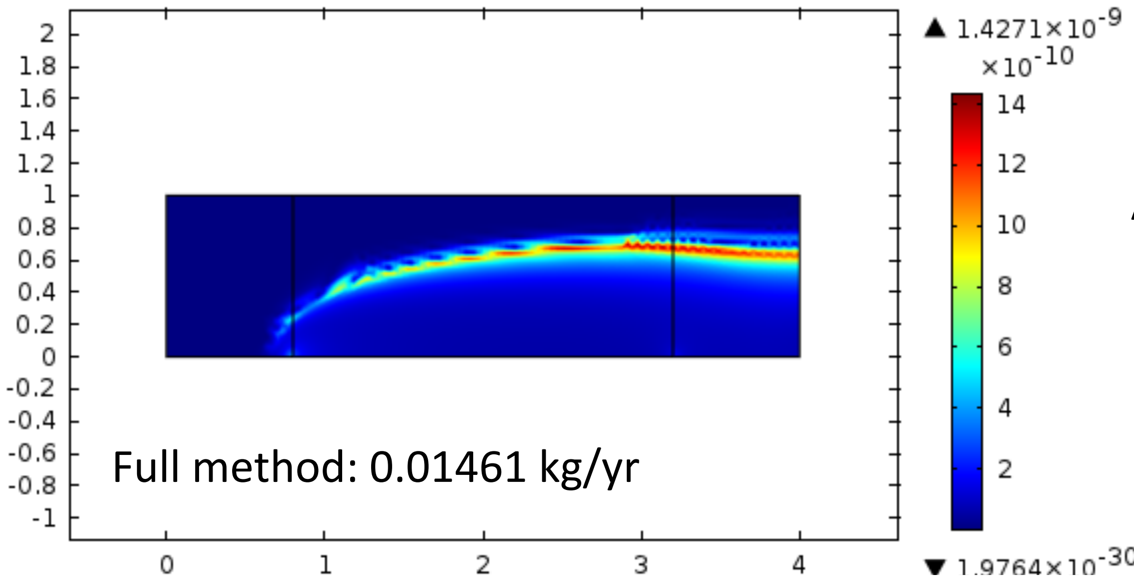
Concentration profile, vs distance from bentonite



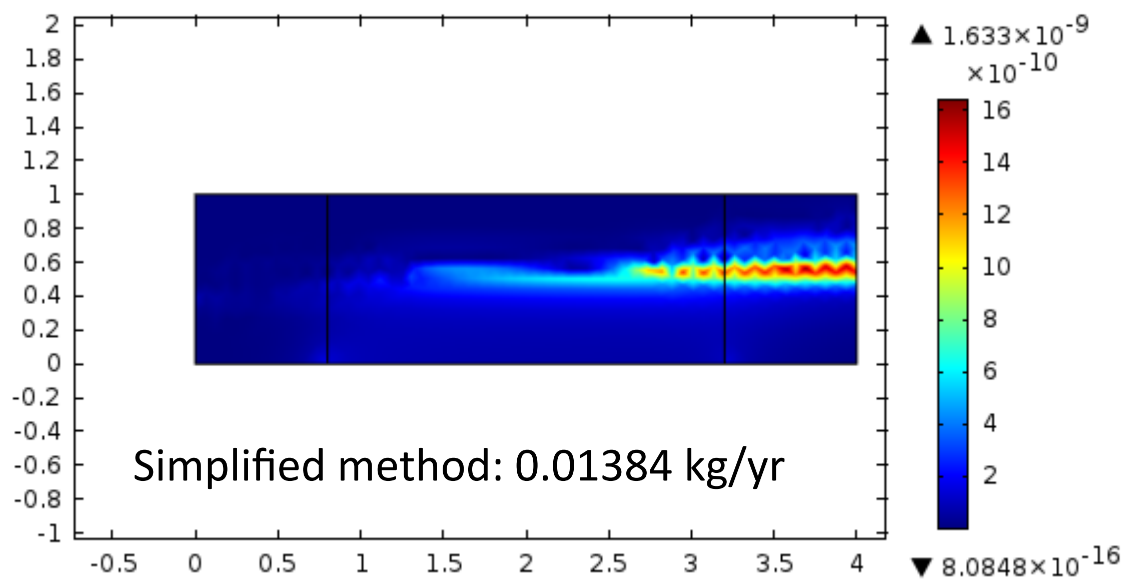

Flowrate vs distance from bentonite



# Compare Full and Simplified method




U=32 m/yr
Aperture=1 mm
Lx=2.4 m



# Simplifications

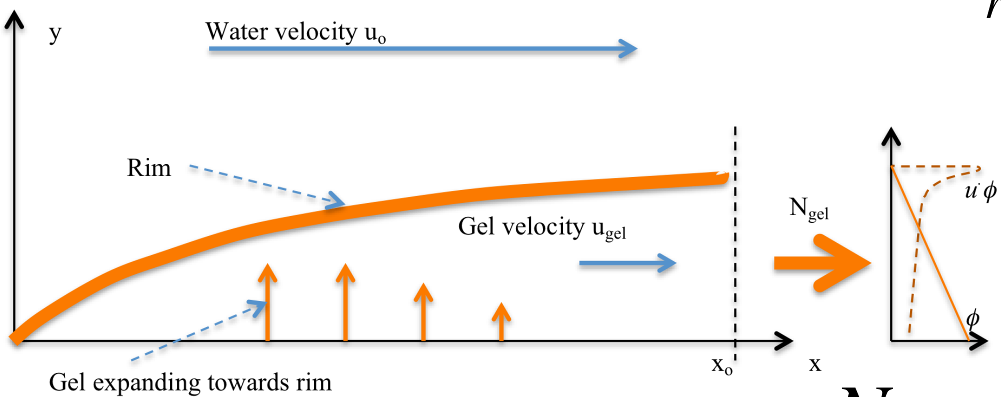
- Isotropic Hydraulic conductivity
- Anisotropic Hydraulic conductivity

Bentonite release kg/yr

| Na concentration | Isotropic K | Anisotropic K |
|---|---|---|
| 0.1 nM | 0.030 | 0.027 |
| 1.0 mM | 0.036 | 0.032 |
| Alpha | 1.12 | 1.12 |

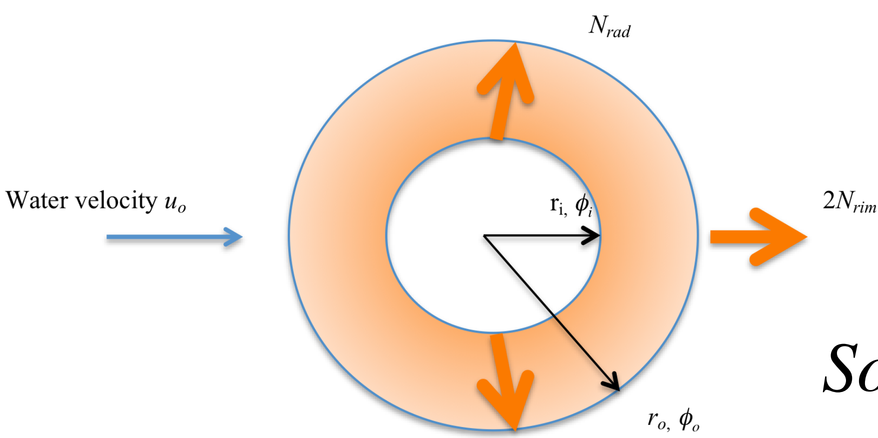
# Combine rim and expansion models

$$N_{rim} \propto f(\phi_i)\delta_{frac}\sqrt{x}$$




$$N_{rad} = \frac{2\pi\delta_{frac}}{\ln(r_o / r_i)} D(\phi_o - \phi_i)$$

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




$$Solve \quad 2N_{rim}(r_i) = N_{rad}(r_i) \quad for\, r_i$$

Thank you for your attention