Modelling smectite loss from a source

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Chemical Engineering and Technology, KTH
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Acknowledgements
The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement n° 295487

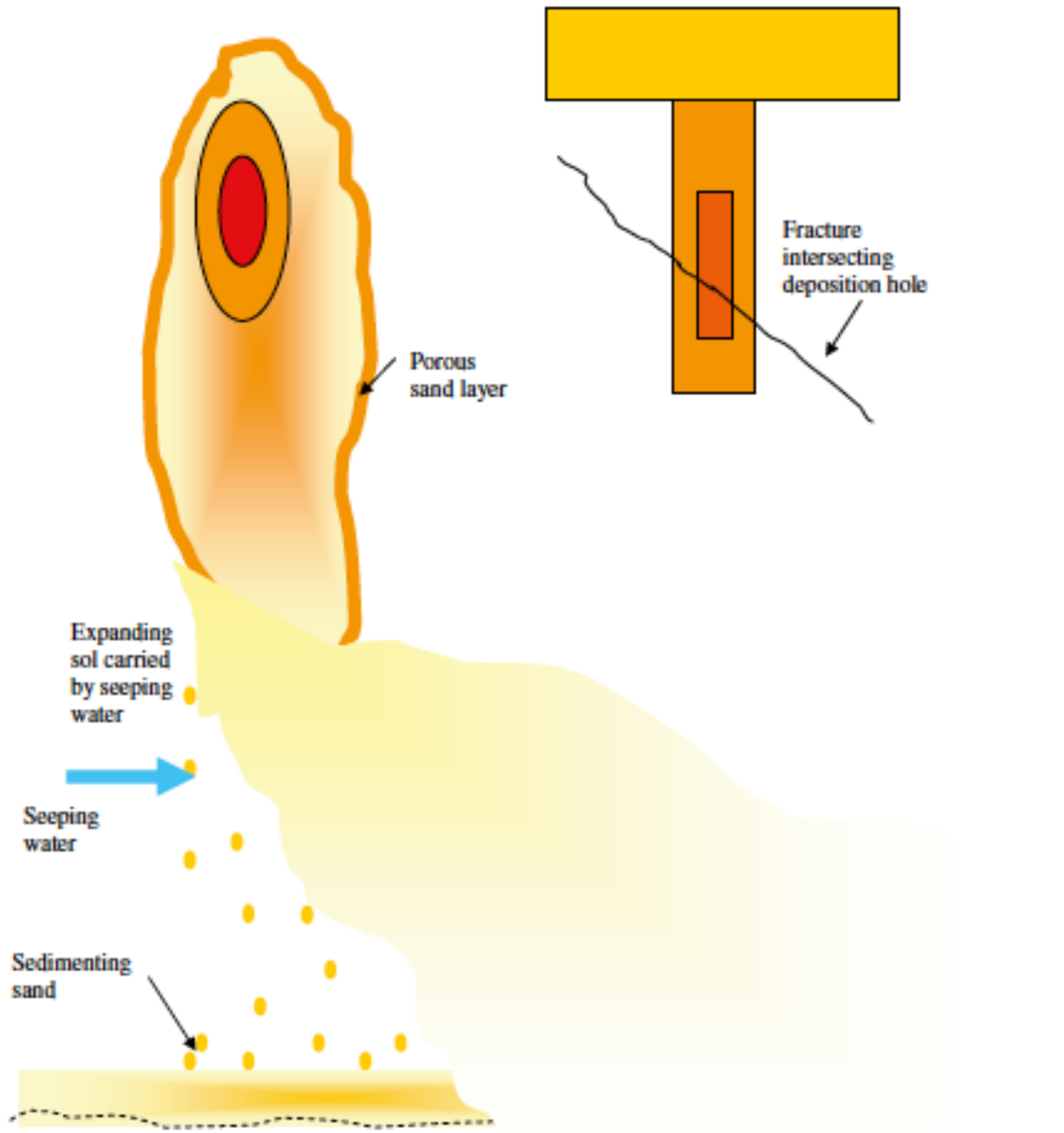
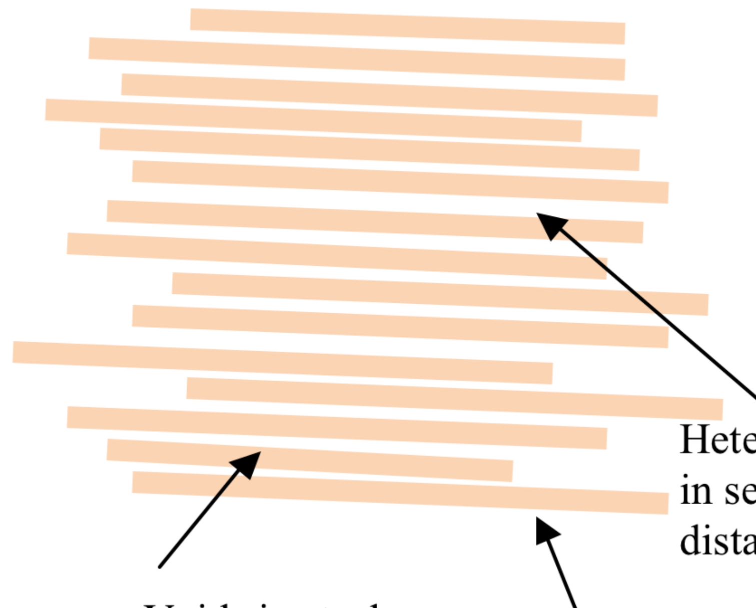
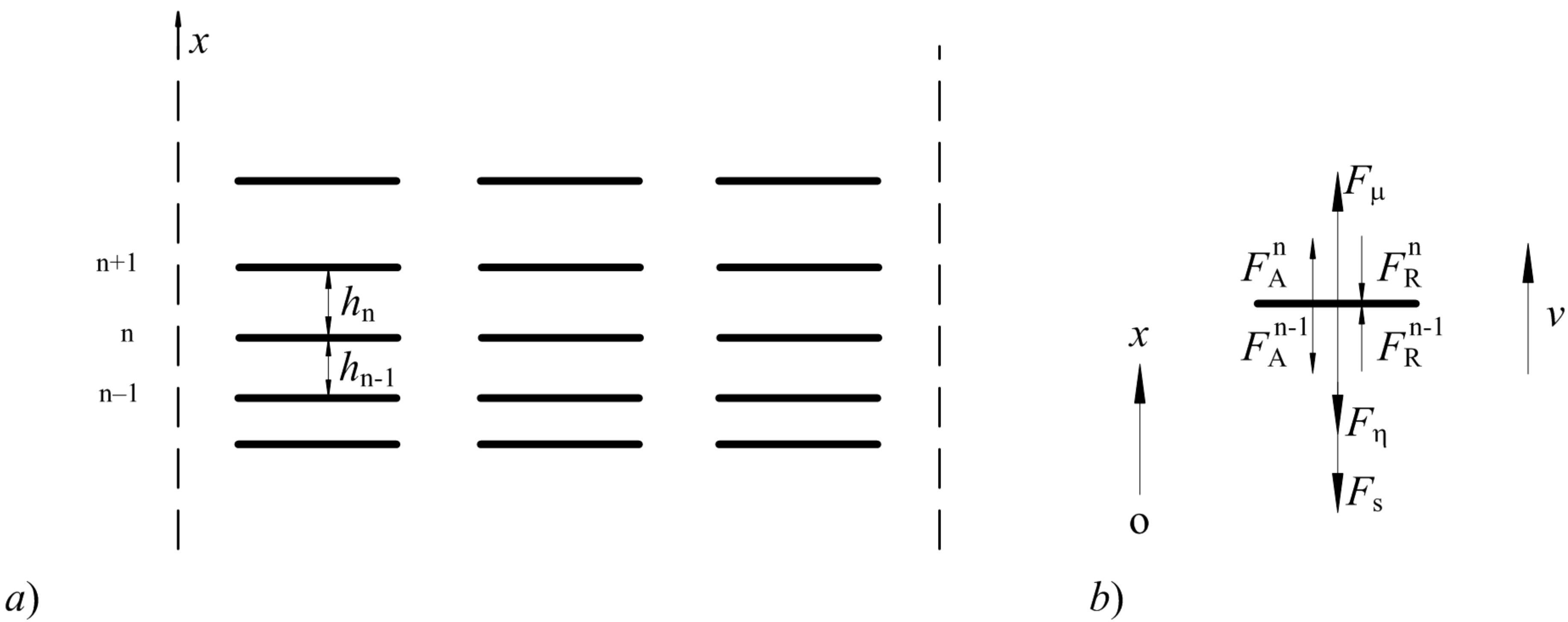


Figure 3-3. Cartoon of how a sand region could develop in the fracture around a deposition hole and that it may be breached and sediment away in the lower parts of the fracture.

Expanding stacks, basis for our dynamic model for gel expansion



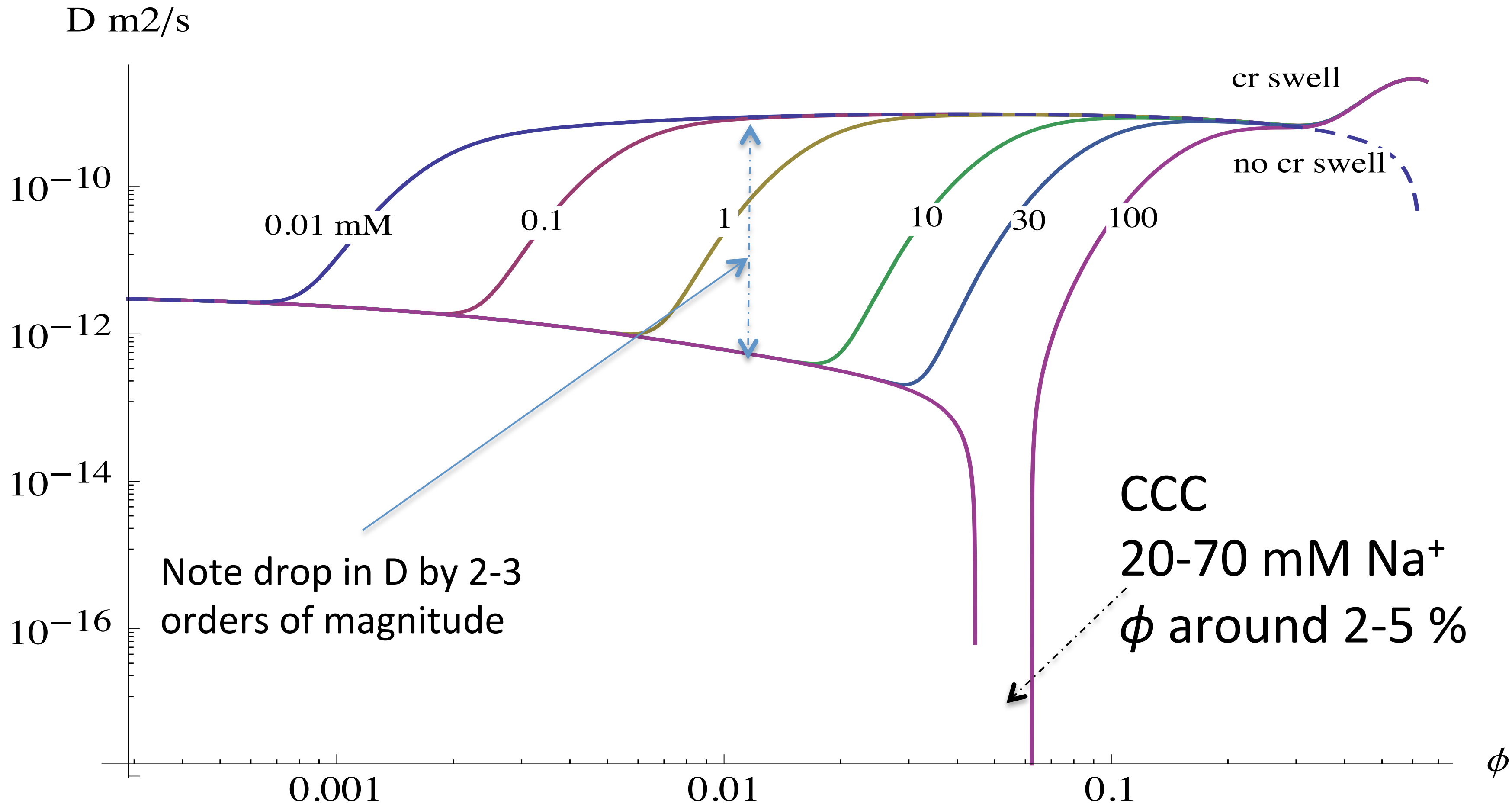
Swelling of parallel sheets



Force balance leads to rate of expansion of paste described by

$$\frac{\partial\ \phi}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(D(\phi) r \frac{\partial \phi}{\partial r}\right)$$

Diffusivity function



Swelling of Na exchanged bentonite in 0.5 mM $CaCl_2$ Validation- Experiments (NMR) and prediction

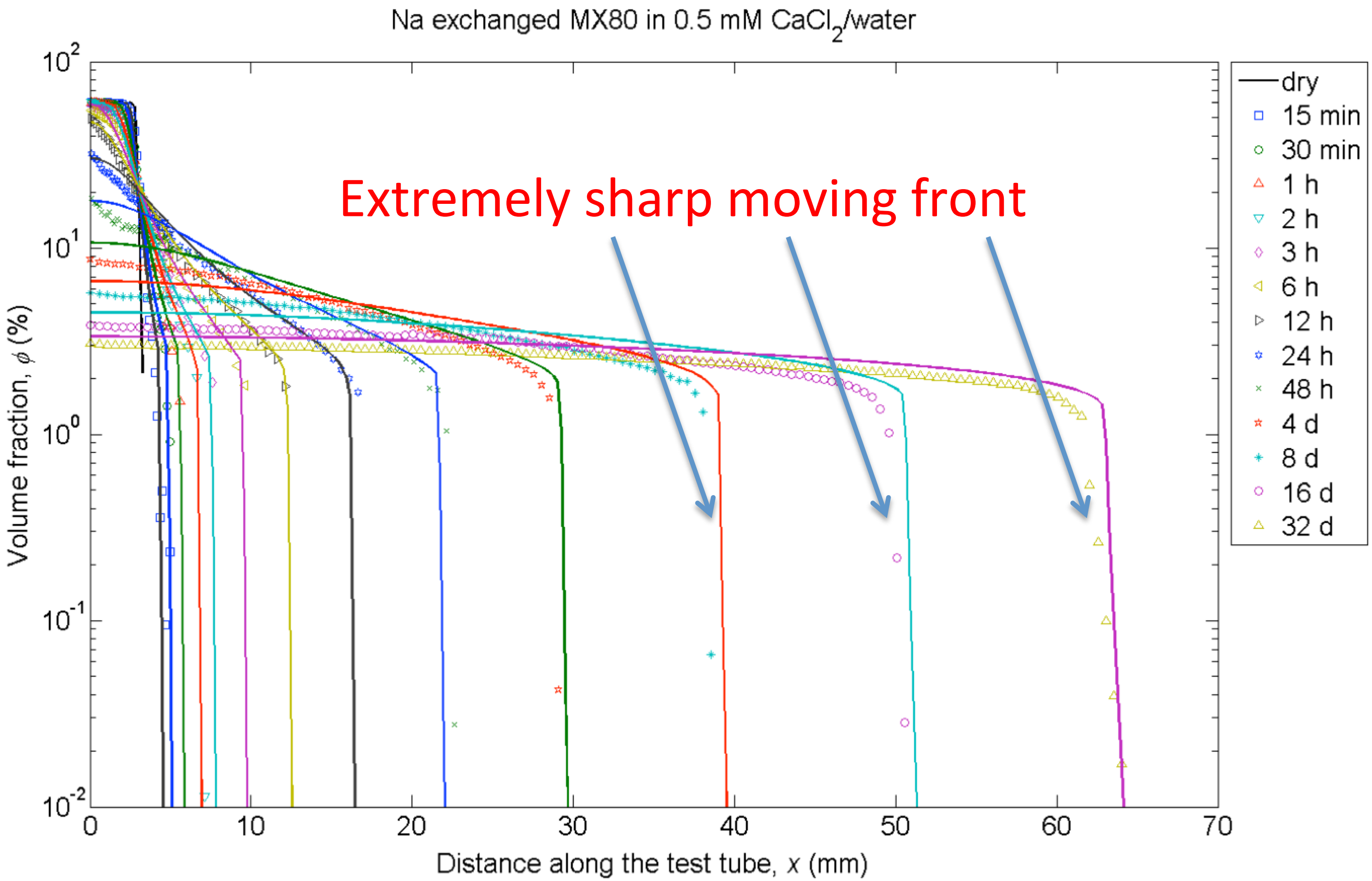
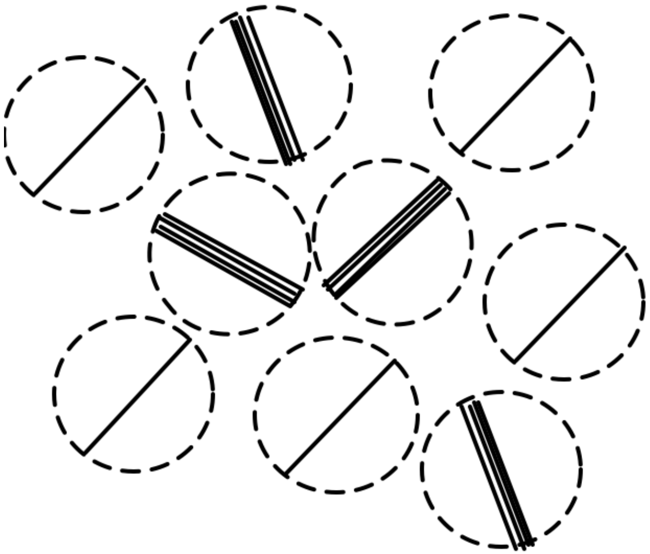
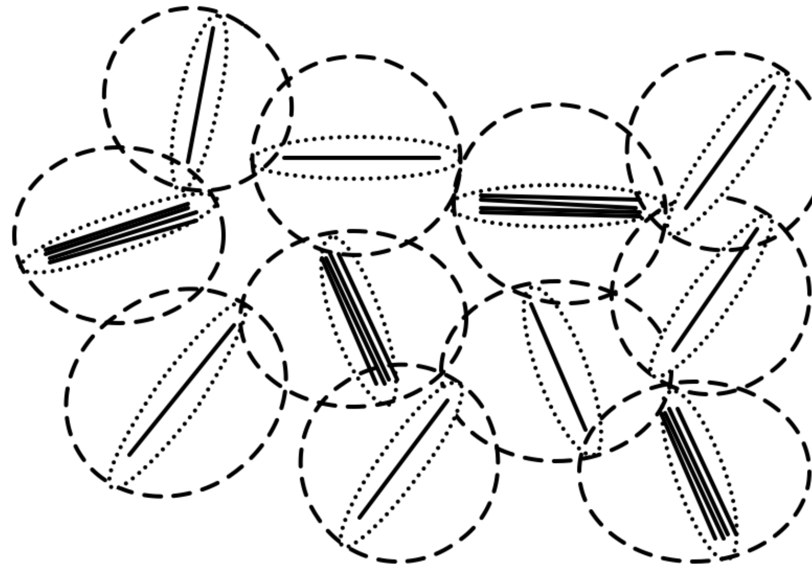


Figure 6.23. Sodium exchanged bentonite in 0.5 mM $CaCl_2$. Logarithmic scale

Co-volume notion- Rotation



Thin diffuse double layer, co-volumes do not overlap

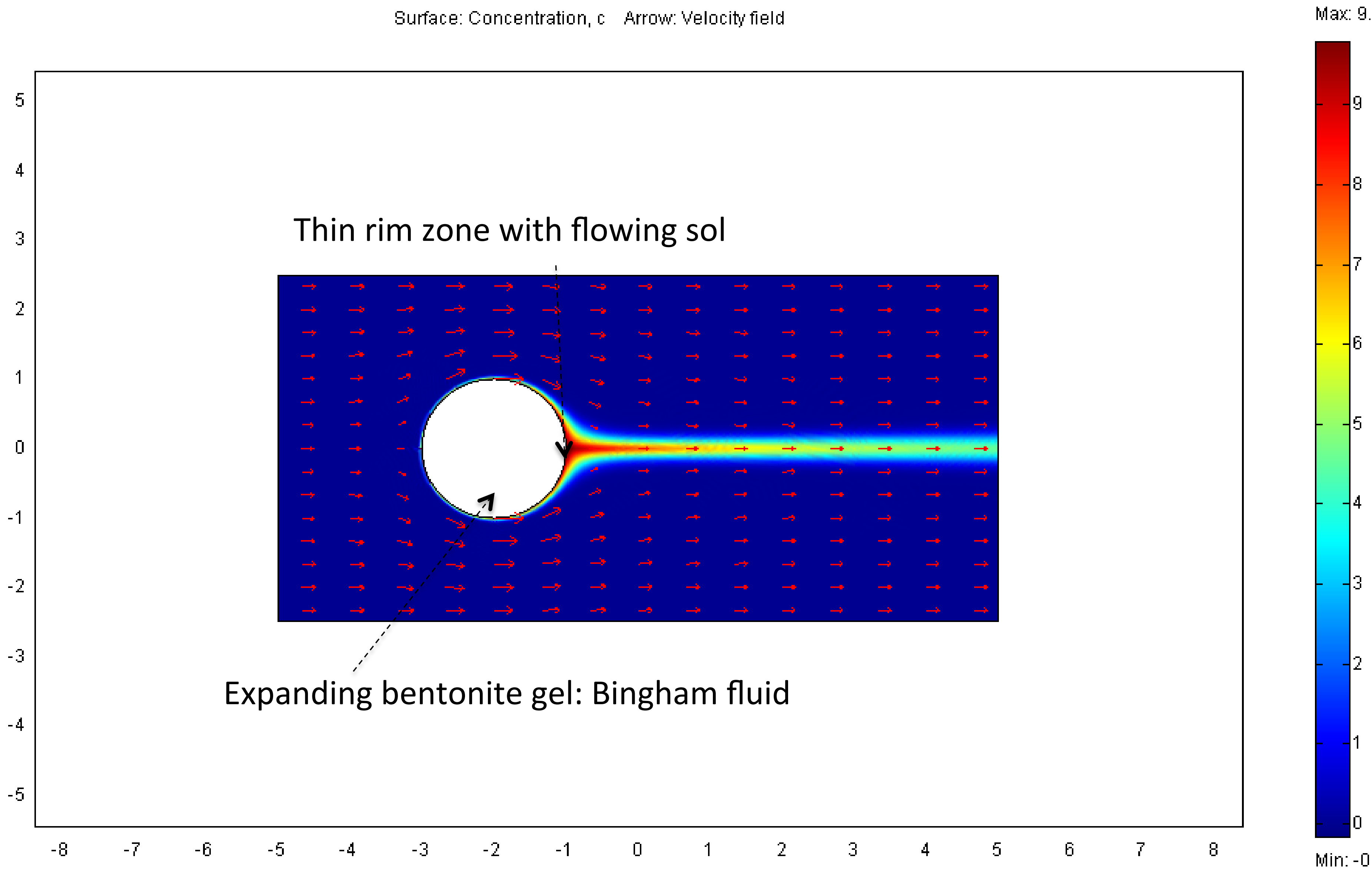


Large diffuse double layer, co-volumes overlap

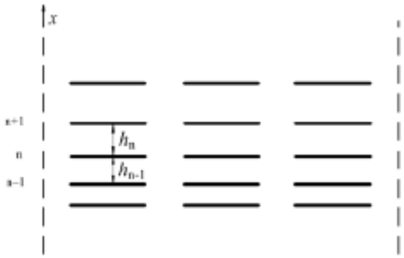
Used to determine viscosity of sol by fitting to experiments

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

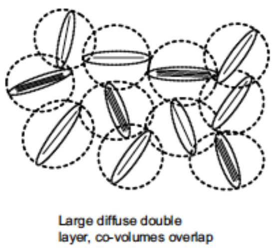
Erosion by sol loss to water



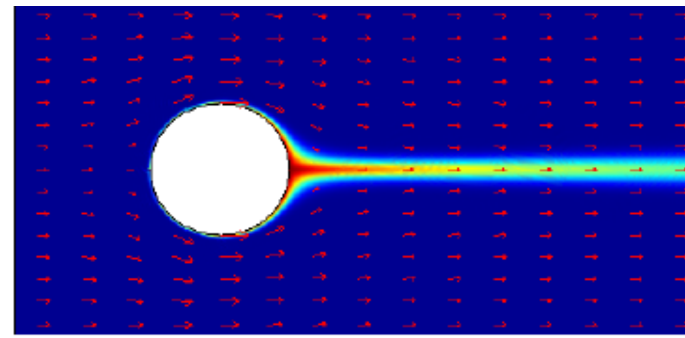
Dynamic model: Summary of processes

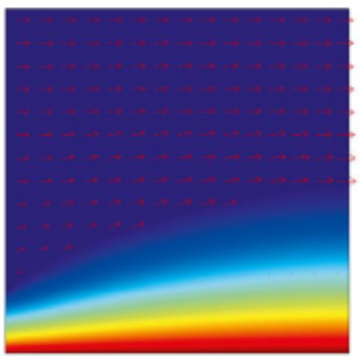


Expansion of
rigid gel.
Viscosity “
infinite



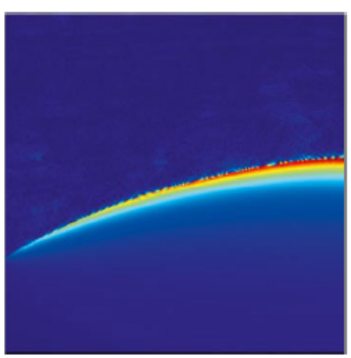
Starting
rotation.
Viscosity of sol
drops, Sol flows





Colloidal particles
diffuse into
seeping water.
Concentration
Picture of rim
zone

Viscosity of sol drops
from 10* water to
water in rim zone

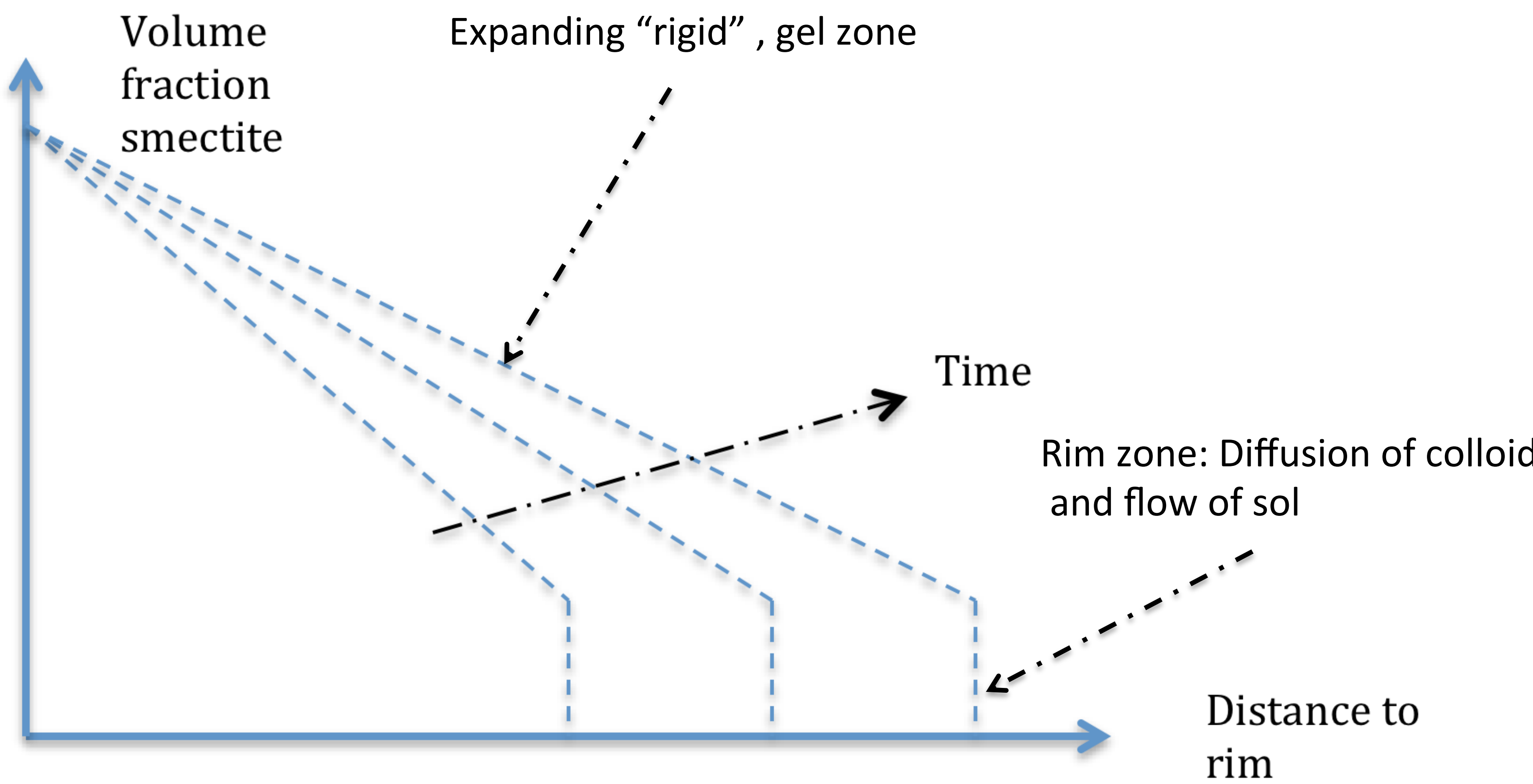


Most flux in thin zone

Interface to rigid gel

Sol flows.
Flux picture
of rim zone

Erosion front, rim, expands w. time. Standard finite element/volume/difference methods cannot follow this well



Two ways of solving the equations

- Simultaneous solution of all coupled eqs.
  - Expansion of paste at rim
  - Formation and flow of sol
  - Diffusion and ion exchange of the different ions
- Two region different techniques to solve
  - The expanding gel up to the rim (sharp front)
  - The loss at the rim
  - Solve the two eqs. coupled

Rim region model, loss N_{rim} at x

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

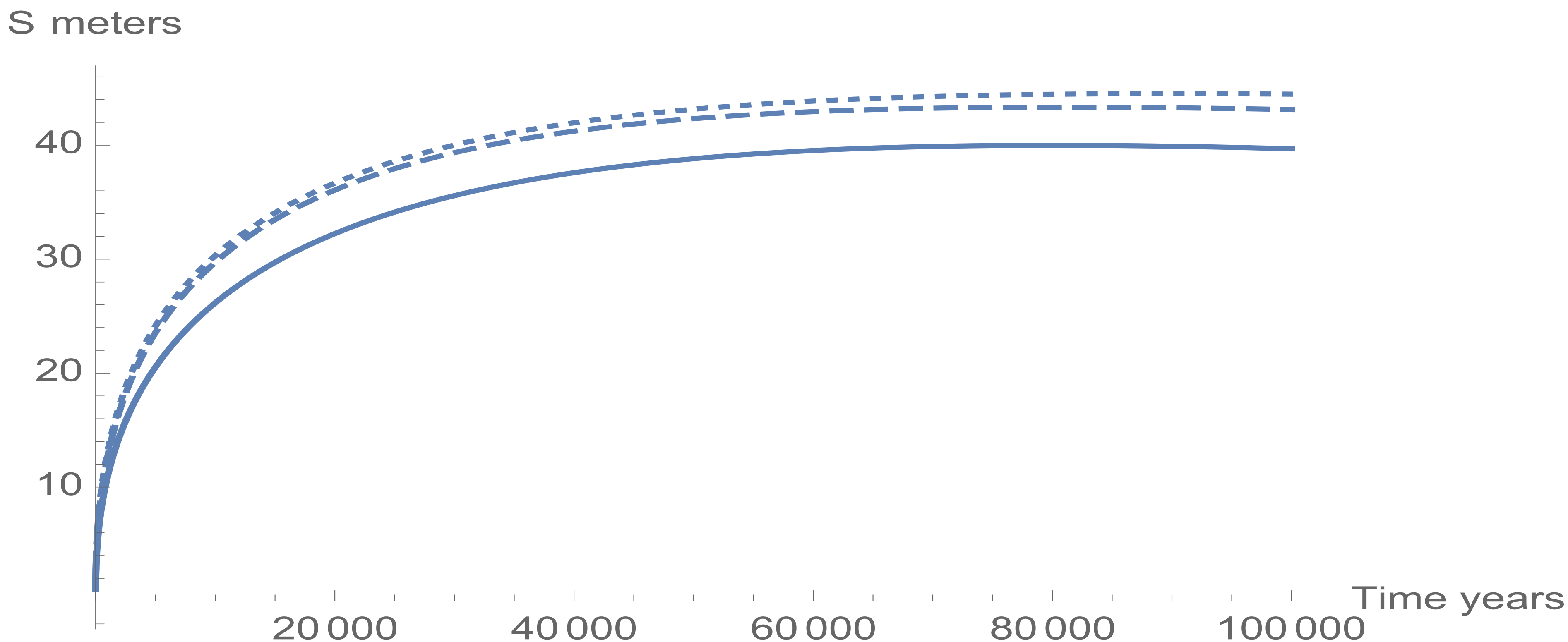
$$N_{rim}^{DL} = \int_0^{\infty} \frac{\phi(z)}{\eta_r(\phi(z))} dz$$

From solution of
Rim zone model

If $\eta_r = 1$ and $D = D_R = constant$

$$N_{rim} = \rho_s \delta_{fr} \phi_R \frac{2}{\sqrt{\pi}} \sqrt{D_R\, x\, u_o}$$

Expansion of rim, Loss at rim accounted for



Expansion of the rim-border for c=0.1 mM and $u_o=10^{-5}$ *m/s, initial* $\phi i=0.574$*,*

Validation

Bentonite swelling and erosion. The 2-region model. Modelling Schatz et al. (2012) experiments

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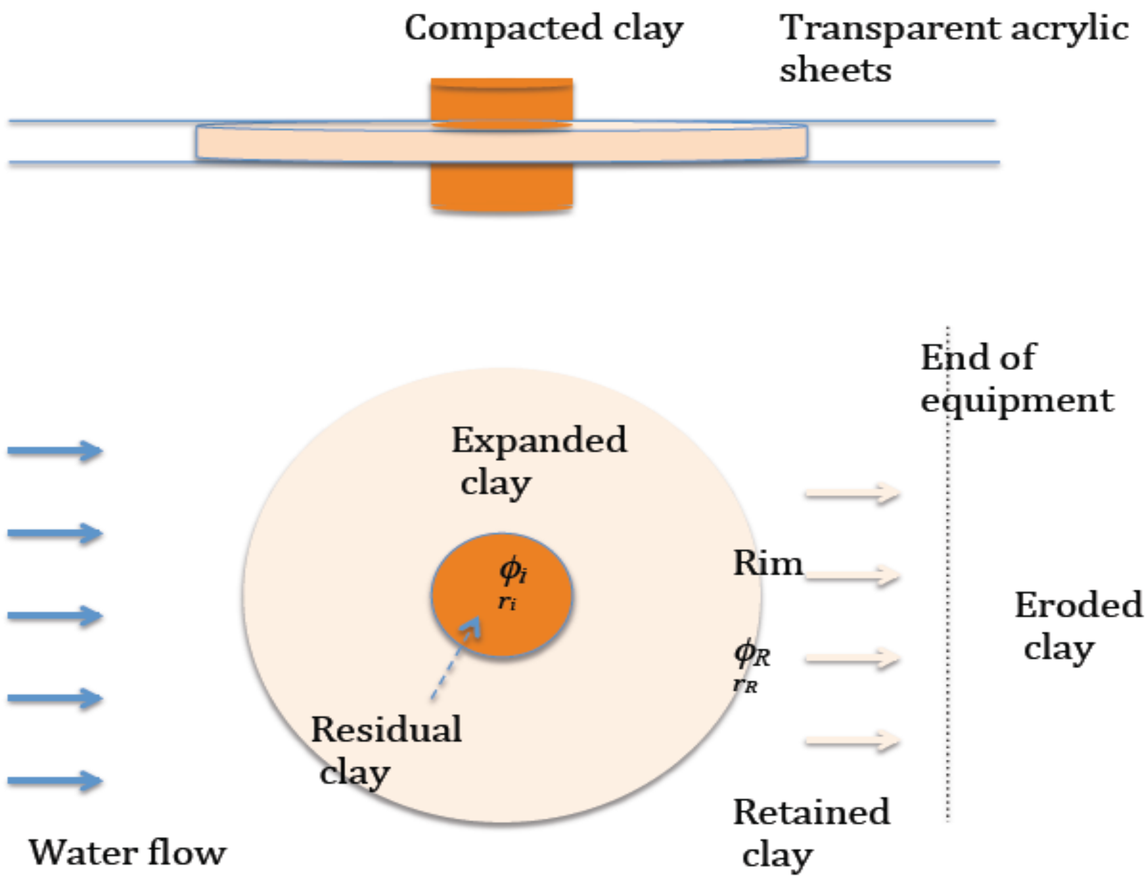
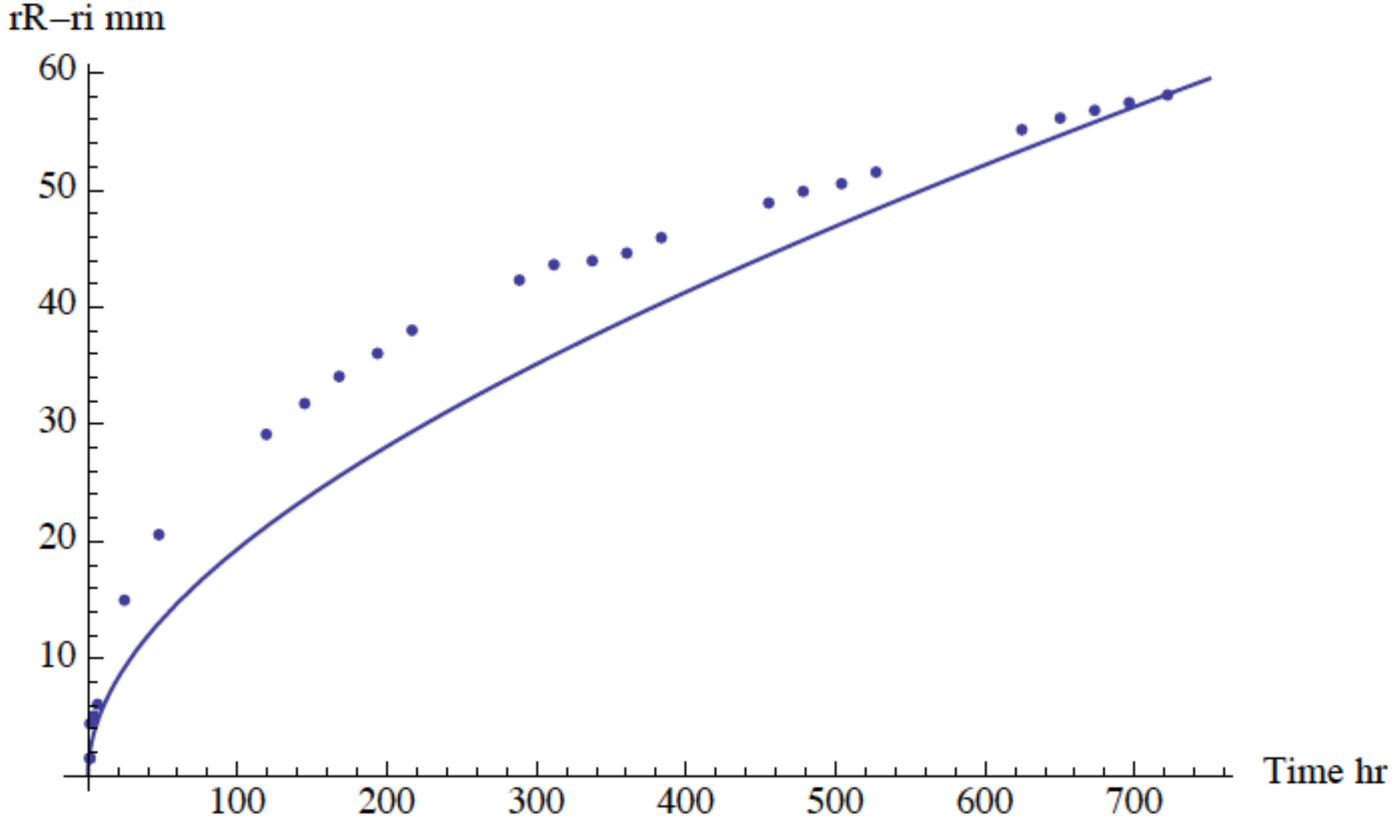
Schatz, T., Kanerva, N., Martikainen, J., Sane, P., Olin, M., Seppälä, A and Koskinen, K., 2012, Buffer Erosion in Dilute Groundwater. Posiva Report 2012-44 (2012).

Schatz et al. (2012) experiments

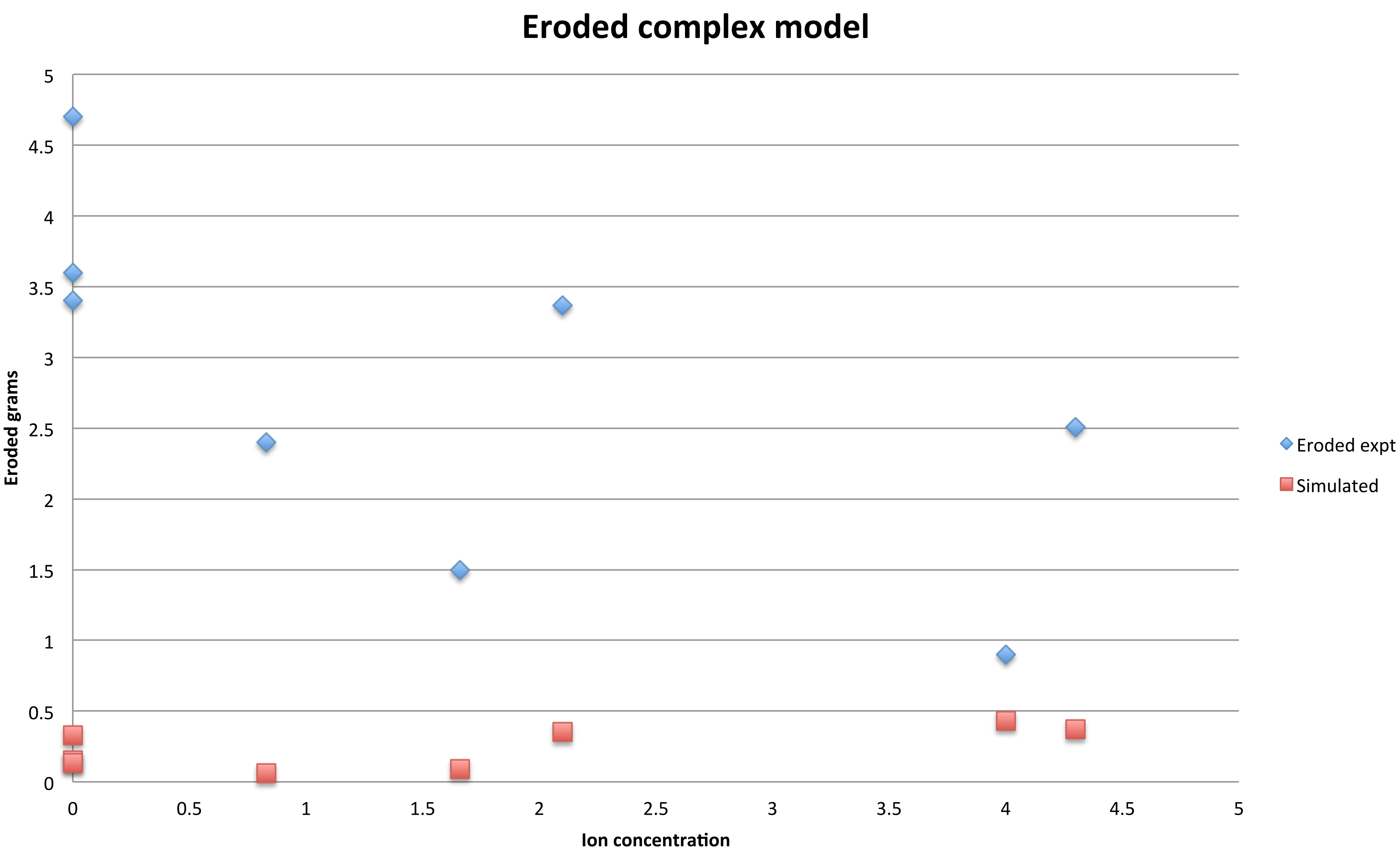


Schatz, T., Kanerva, N., Martikainen, J., Sane, P., Olin, M., Seppälä, A and Koskinen, K., 2012, Buffer Erosion in Dilute Groundwater. Posiva Report 2012-44 (2012).

Just expansion no flow, DI water



Predicted erosion with 2-region model



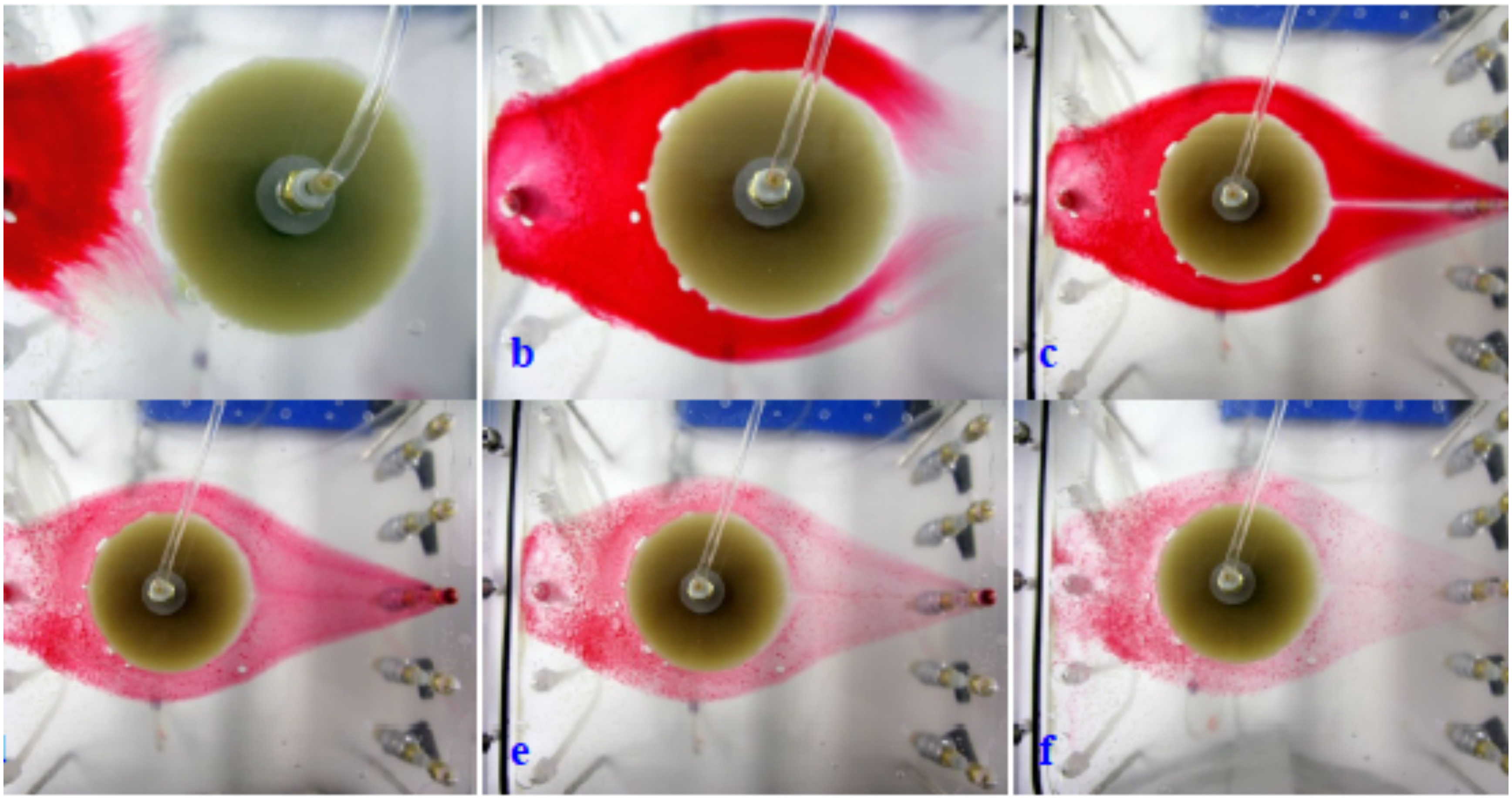
Obviously this is not a good prediction

Model is wrong or model does not account for some mechanism(s)

Agglomeration to flocs, Low ionic strength water

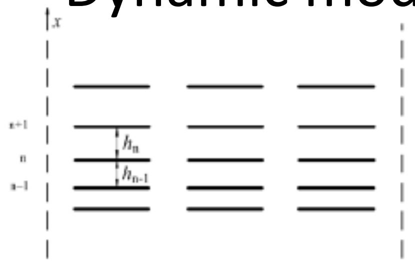
Schatz et al. (2012), Buffer Erosion in Dilute Groundwater. Posiva Report 2012-44.

Expanded gel & flow pattern

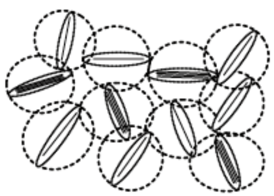


Schatz et al. (2012), Buffer Erosion in Dilute Groundwater. Posiva Report 2012-44.

Dynamic model

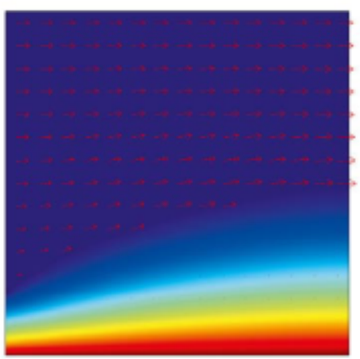


Expansion of rigid gel.
Viscosity “ infinite

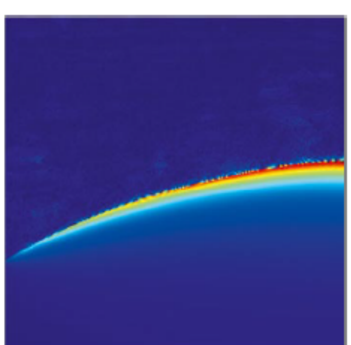


Large diffuse double layer, co-volumes overlap

Starting rotation.
Viscosity of sol drops

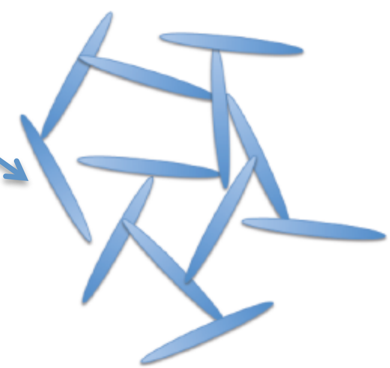


Colloidal particles diffuse into seeping water.
Concentration
Picture of rim zone

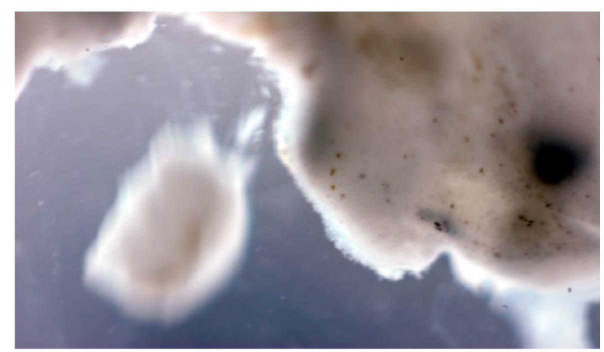


Sol flows.
Flux picture
Of rim zone

Dynamic model with floc formation



Flocs form. Can sediment.
Floc slurry viscosity near water.



Rim zone model III

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

$$N_{rim}^{DL} = \int_0^{\infty} \frac{\phi(z)}{\eta_r(\phi(z))} dz$$

If $\eta_r = 1$ and $D = D_R = constant$

$$N_{rim} = \rho_s \delta_{fr} \phi_R \frac{2}{\sqrt{\pi}} \sqrt{D_R\, x\, u_o}$$

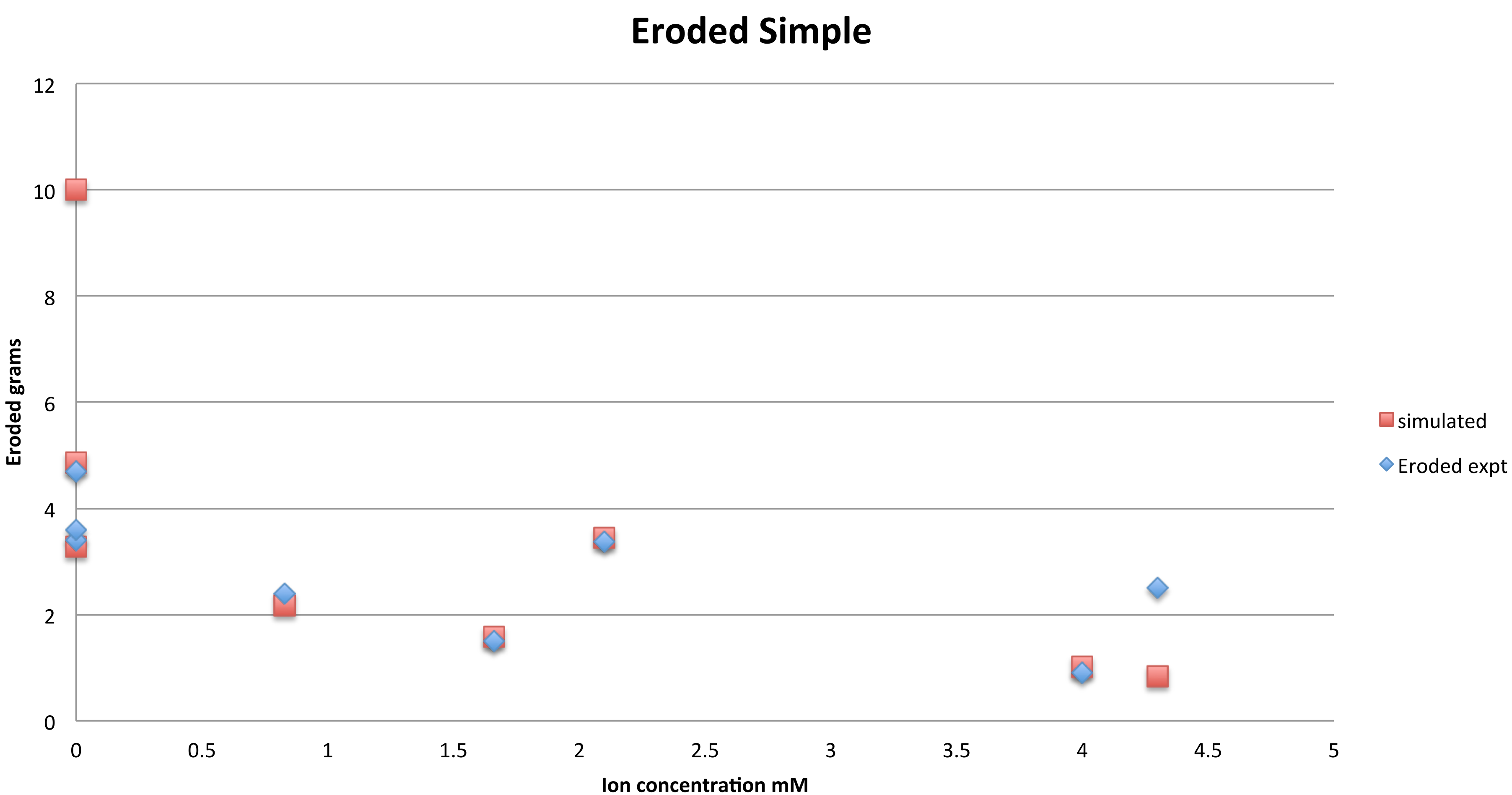
Changes and simplifications of model

- Floc slurry viscosity ≈ as water
- Volume fraction at rim ϕ_R indep. of ion conc.
- Loss rate expression simplifies to

$$N_{rim} = \rho_s \delta_{fr} \phi_R 2\sqrt{D_R r_R u_o}$$

But ϕ_R *now is an adjustable parameter,*
D_R *– diffusivity at rim- is still from Diffusivity function and it depends on* c_{ion}

Simulated erosion with Simple 2-region model ϕ_R=0.015



Also r_R, Extruded, Residual, Retained and Eroded masses agree quite well

Smectite loss by flocculation and gravity

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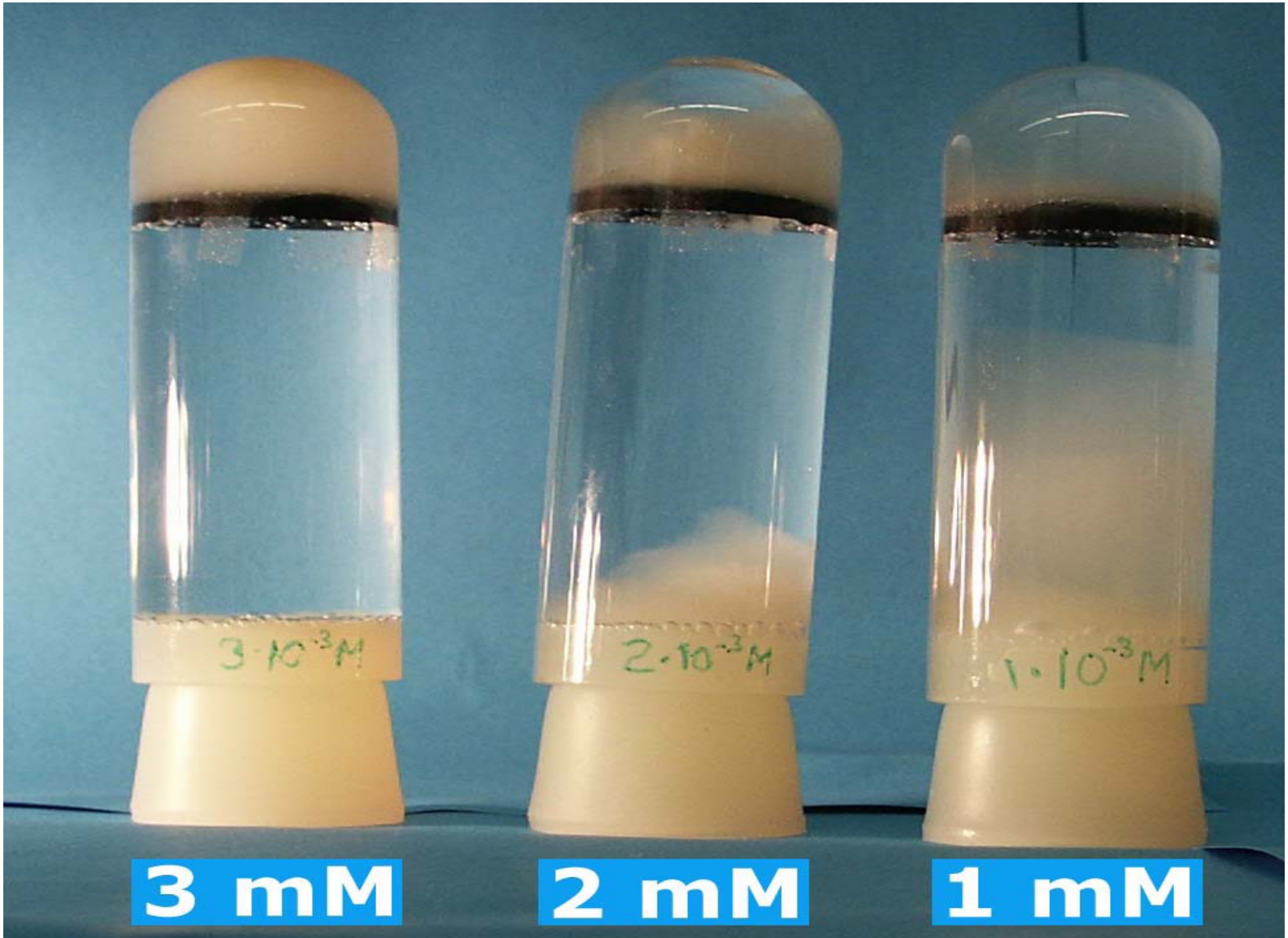
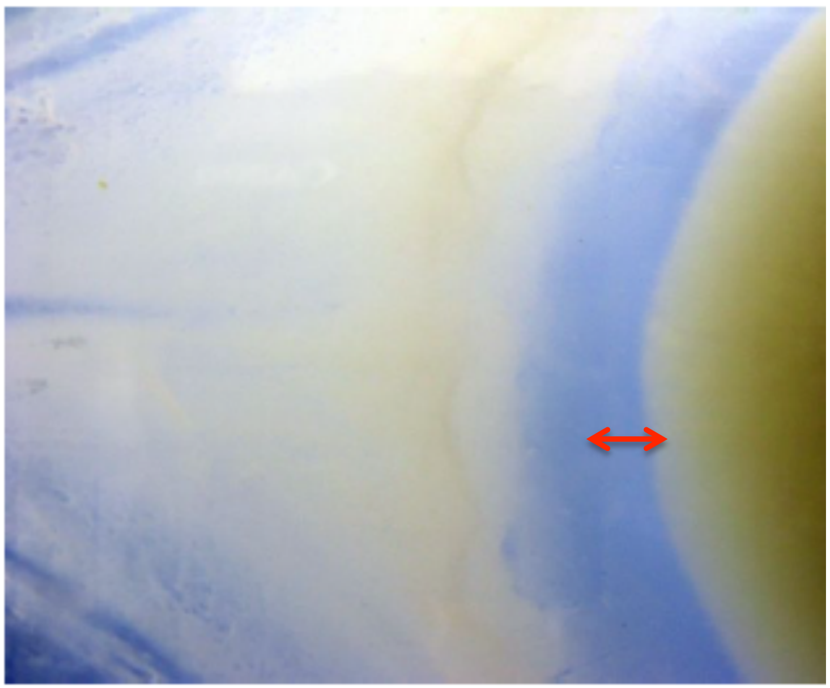
Flocs fall through fine filter, 10 μm



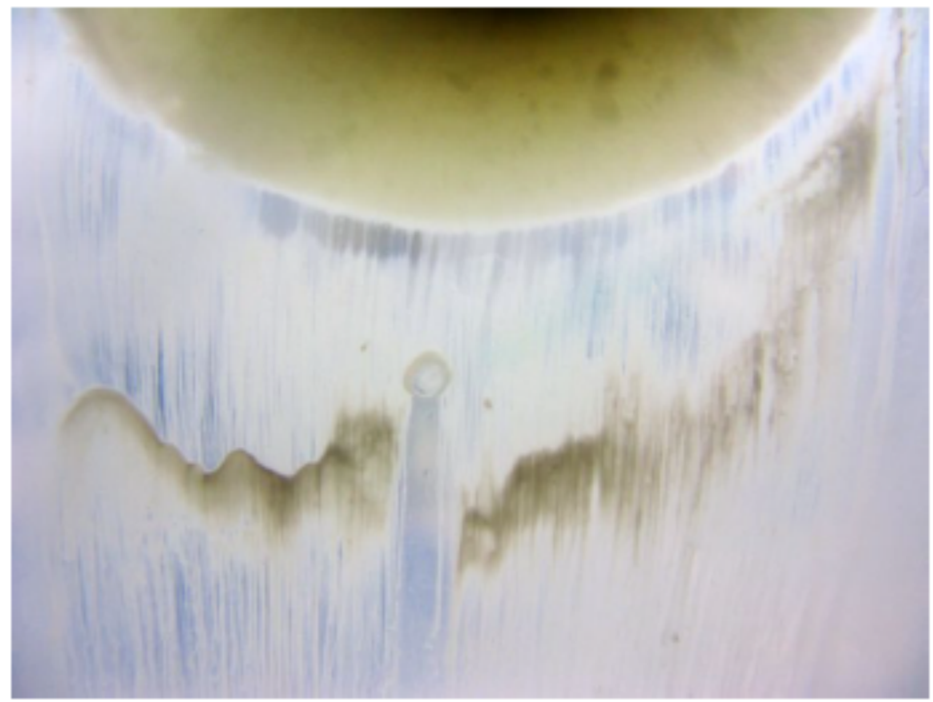
Schatz et al. (2012) erosion experiments

50/50 calcium/sodium montmorillonite in Di

Formation of flocs



Gravity pulling off flocs when slit is vertical



Schatz, T., Kanerva, N., Martikainen, J., Sane, P., Olin, M., Seppälä, A and Koskinen, K., 2012, Buffer Erosion in Dilute Groundwater. Posiva Report 2012-44 (2012).

Model w. small spheres

Sedimentation rate of spheres, Stokes law

$$v_{sph} = \frac{2}{9\mu_W} r_{sph}^2 \left(\varrho_{sph} - \varrho_W\right) g$$

$$\varrho_{sph} = \phi\, \varrho_{smec} + (1-\phi)\, \varrho_w$$

$$\varrho_{\#} = \frac{1}{r_{sph}^3 n_{rS,v}\, n_{rS,h}^2}$$

$$N_{smec} \propto \frac{1}{n_{rS,v}\, n_{rS,h}^2}\, r_{sph}^2 \delta W_{AF}$$

Maximum loss as spheres

Largest sphere diam = aperture

Note cubic dependence on aperture

$$N_{smec} = fr\,\frac{\pi\delta^3}{108\mu_W}\left(\varrho_{sph} - \varrho_W\right) g\phi\varrho_{smec}W_{AF}$$

fr is fraction of maximum # of spheres per volume

Model with Coins- Friction against walls

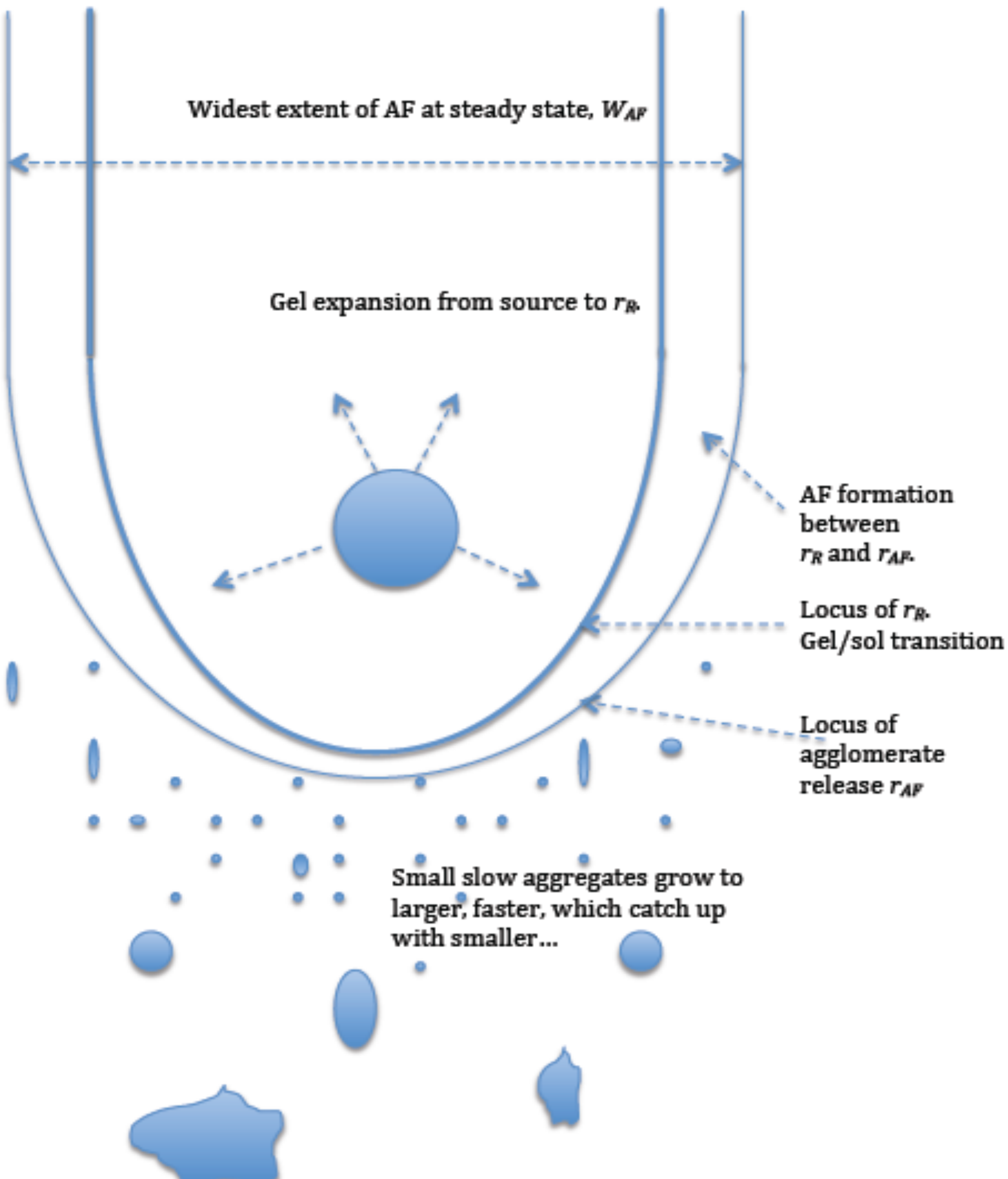
Sedimentation rate of “coin” or viscous agglomerate fluid AF, -> Cubic law

$$N_{smec,max,coin} = \frac{\pi\delta^3}{12\mu_{agg}}(\varrho_{sph} - \varrho_W)g\phi\varrho_{smec}W_{AF}$$

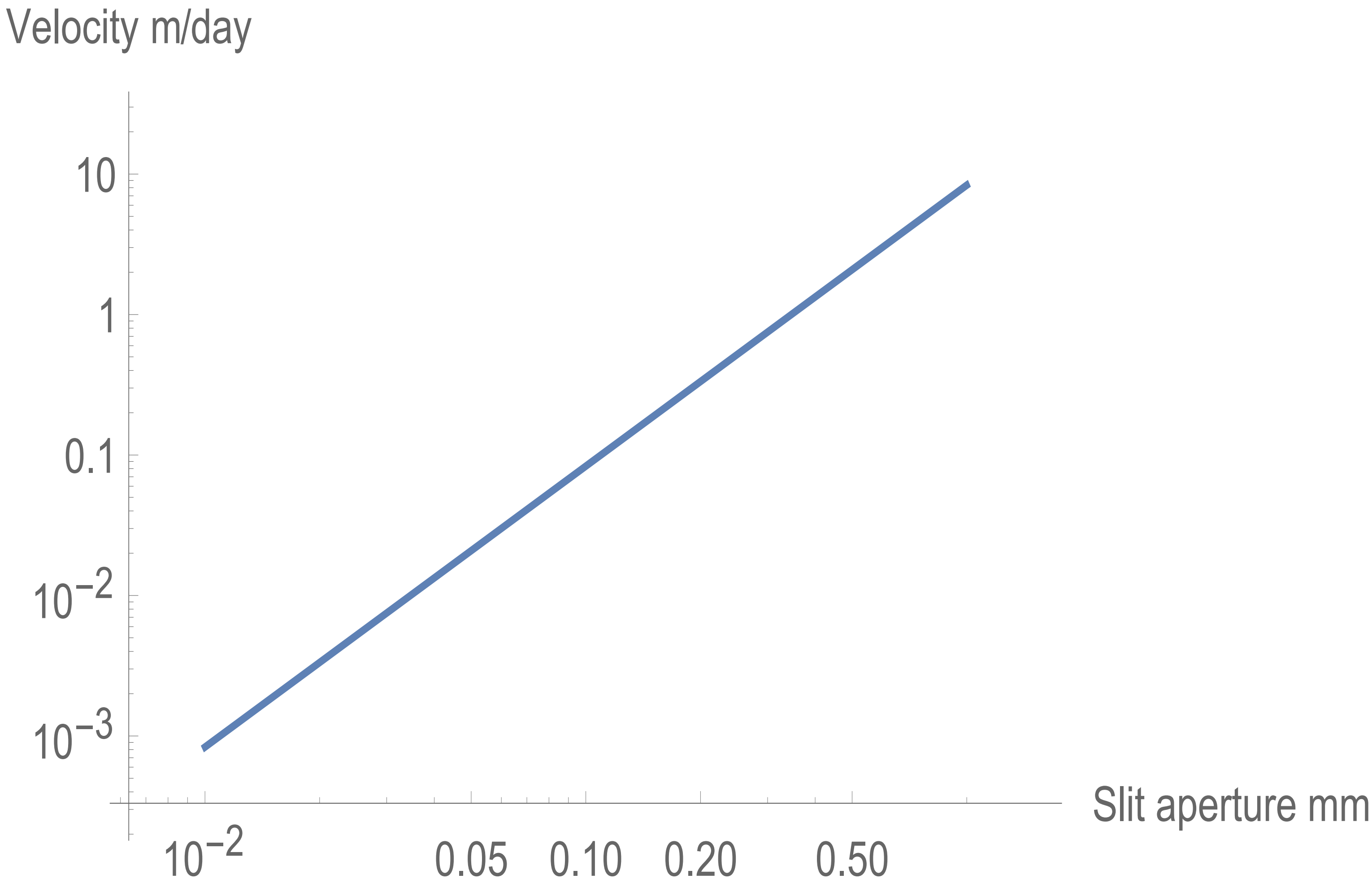
“Coin” filling whole width of source W_{AF}

$$\mu_{agg} \cong 10 * \mu_W$$

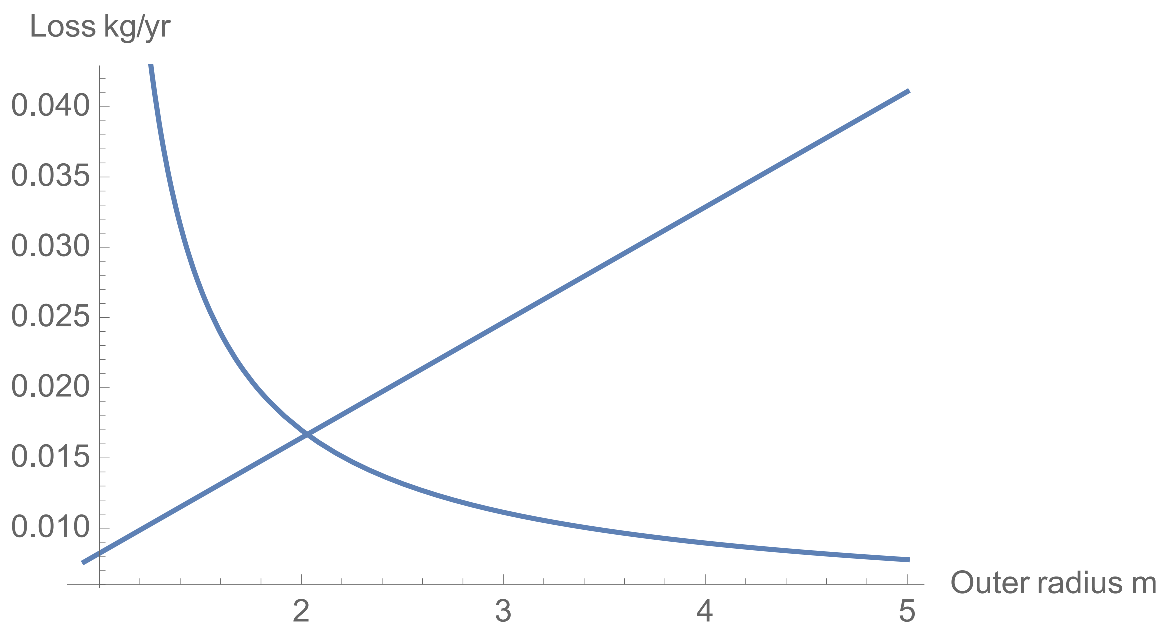
Loss of smectite by floc sedimentation



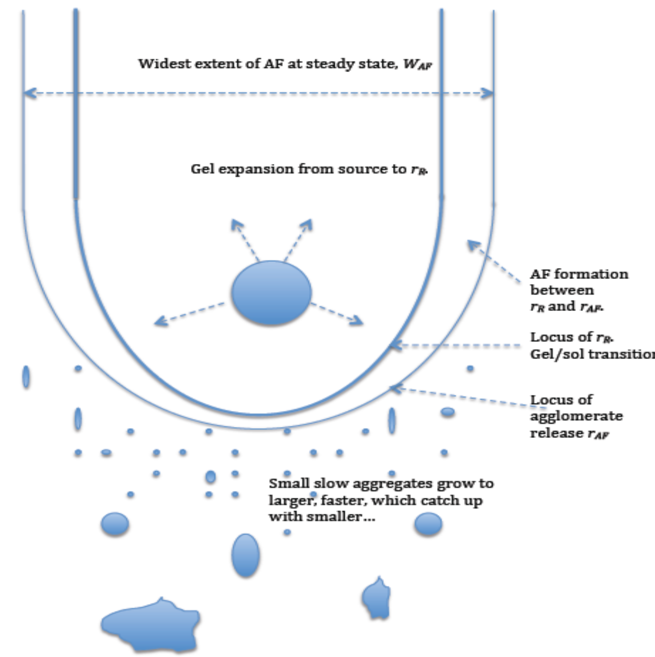
Sedimentation velocity of large coin-like agglomerates with 1% by volume smectite in a vertical slit vs. slit aperture.



Stabilisation of width of expansion



Aperture 0.1 mm, fr=0.01



Rate of loss from deposition hole N_{PSS} (curved line) and rate of loss by sedimentation N_{smec} (straight line) as function of the radius to the rim

Some queries I

Where does the bentonite end up?

Example 100 kg bentonite loss

Agglomerate volume fraction of bentonite= 0.01
Rock porosity of fractures 10^{-4}

Fills 38 000 m^3 rock
A cube with 34 m sides

Could this be used as an argument against large loss?

Some queries II

- Where does the detritus end up?
- What does the detritus do to the loss of smectite?

Some references on erosion modelling and background reports

SKB reports can be freely downloaded from www.SKB.se
Posiva reports can be freely downloaded from www.Posiva.fi
The reports marked yellow summarise modelling approaches

Liu, L., 2010. Permeability and expansibility of sodium bentonite in dilute solutions. Colloids Surf. A: Physicochem. Eng. Aspects 358 (1–3), 68–78.

Liu L. Neretnieks I., Moreno L., Permeability and expansibility of natural bentonite MX-80 in distilled water, Physics and Chemistry of the Earth 36 (2011) 1783–1791

Liu L., 2011, A model for the viscosity of dilute smectite gels, Physics and chemistry of the earth, 36, p 1792-1798

Liu L., 2013, Prediction of swelling pressures of different types of bentonite in dilute solutions, Colloids and Surfaces A: Physicochem. Eng. Aspects 434 (2013) 303– 318

Liu, L., Moreno, L., Neretnieks, I., 2009a. A Dynamic force balance model for colloidal expansion and its DLVO-based application. Langmuir 25 (2), 679–687.

Liu, L., Moreno, L., Neretnieks, I., 2009b. A novel approach to determine the critical coagulation concentration of a colloidal dispersion with plate-like particles. Langmuir 25 (2), 688–697.

Liu L., Neretnieks I., Moreno L., 2011, Permeability and expandability of natural bentonite MX-80 in distilled water. Physics and Chemistry of the Earth, 36, p 1783-1791

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Moreno L., Neretnieks I., Liu L., 2011, Erosion of sodium bentonite by flow and colloid diffusion, Physics and chemistry of the earth, 36, p 1600-1606

Neretnieks, I., Liu, L., Moreno, L., 2009. Mechanisms and Models for Bentonite Erosion. Swedish Nuclear Fuel and Waste management Co., Technical report, SKB TR-09-35

Neretnieks I., Liu L., Moreno, L., 2010, Mass transfer between waste canister and water seeping in rock fractures. Revisiting the Q-equivalent model, Swedish Nuclear Fuel and Waste management Co., Technical report, SKB TR-10-42

Schatz, T., Kanerva, N., Martikainen, J., Sane, P., Olin, M., Seppälä, A and Koskinen, K., 2012, Buffer Erosion in Dilute Groundwater. Posiva Report 2012-44 (2012).

Reports submitted to BELBaR 2015

1) Bentonite expansion and erosion- Development of a two-region model by Ivars Neretnieks, Luis Moreno and Longcheng Liu

2) Evaluation of some erosion experiments by the two-region model by Ivars Neretnieks, Luis Moreno and Longcheng Liu

3) Release and sedimentation of smectite agglomerates from bentonite gel/sol by Ivars Neretnieks

Thank you for your attention