Modelling slit erosion experiments

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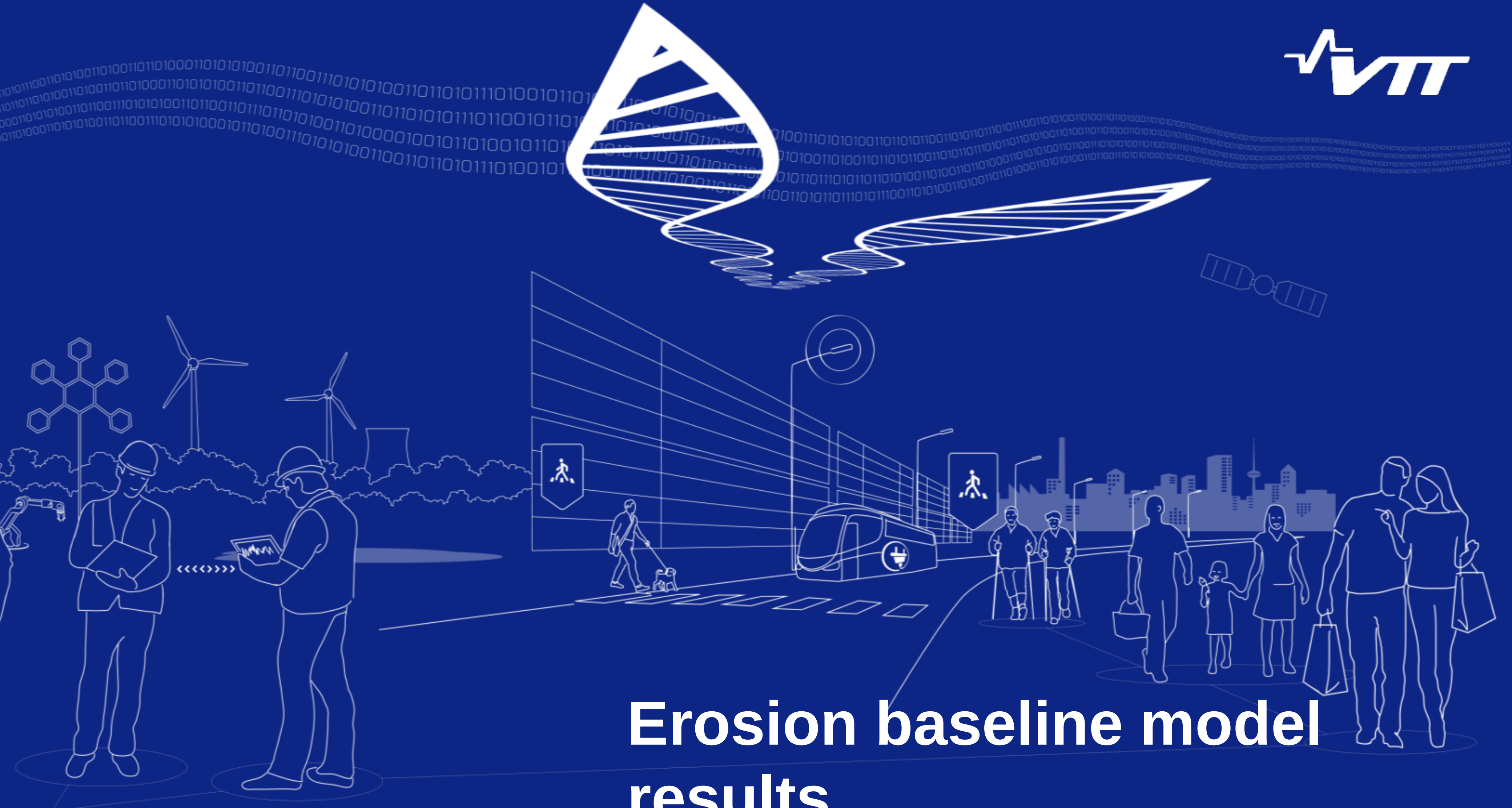


Erosion baseline model results

Model setup & calculated cases

Modified erosion baseline model

- viscosity of gel limited: 700 and 45 000 times the lowest value (correspond to values at 0.025 and 0.1 bentonite volume fractions)
- direct functional relations replaced by polynomial interpolants

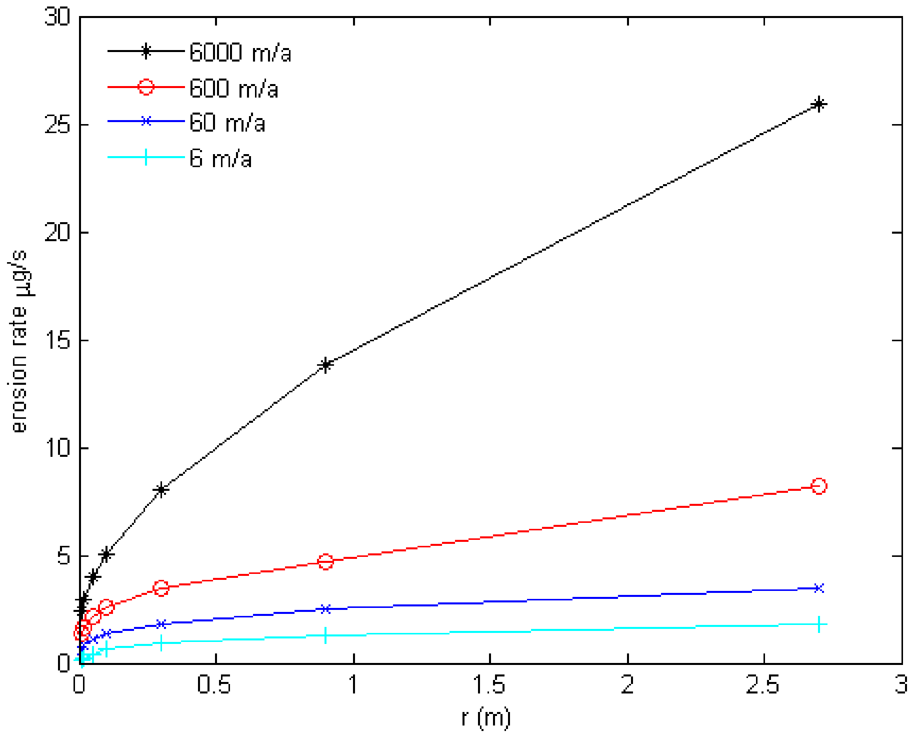
Calculated cases

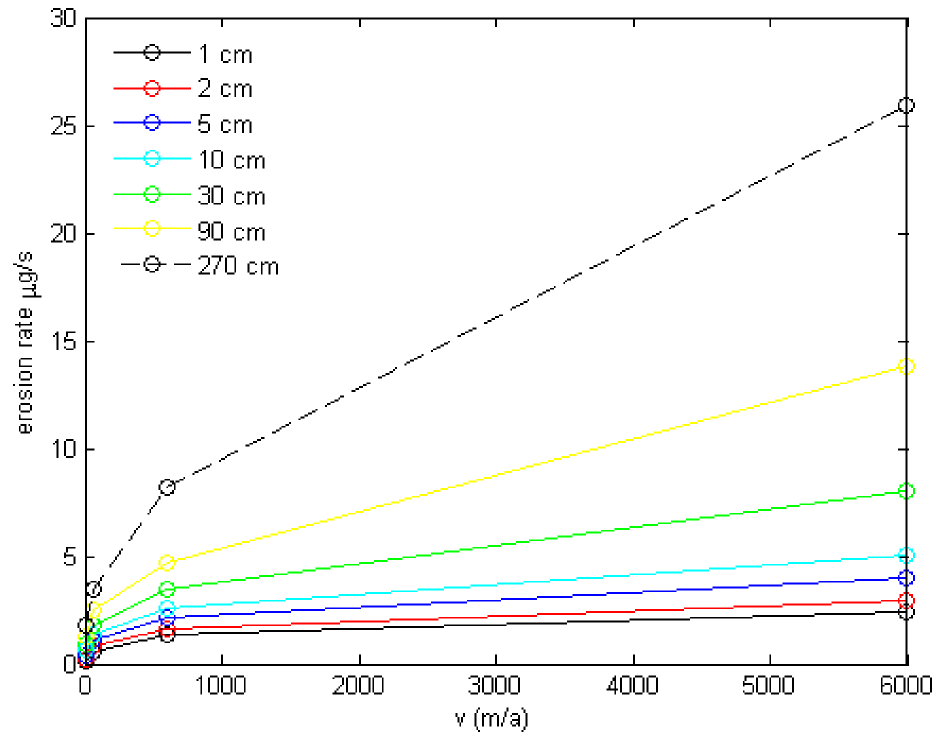
- salinity 0.1 mM
  - flow velocities: 0.6, 6, 60, 600, 6000 m/a
  - radii: 1, 2, 5, 10, 30 and 270 cm
- salinities 0.1 - 30 mM
  - radius 1 cm
  - flow velocity 6000 m/a

Results (1/2): fixed salinity 0.1 mM

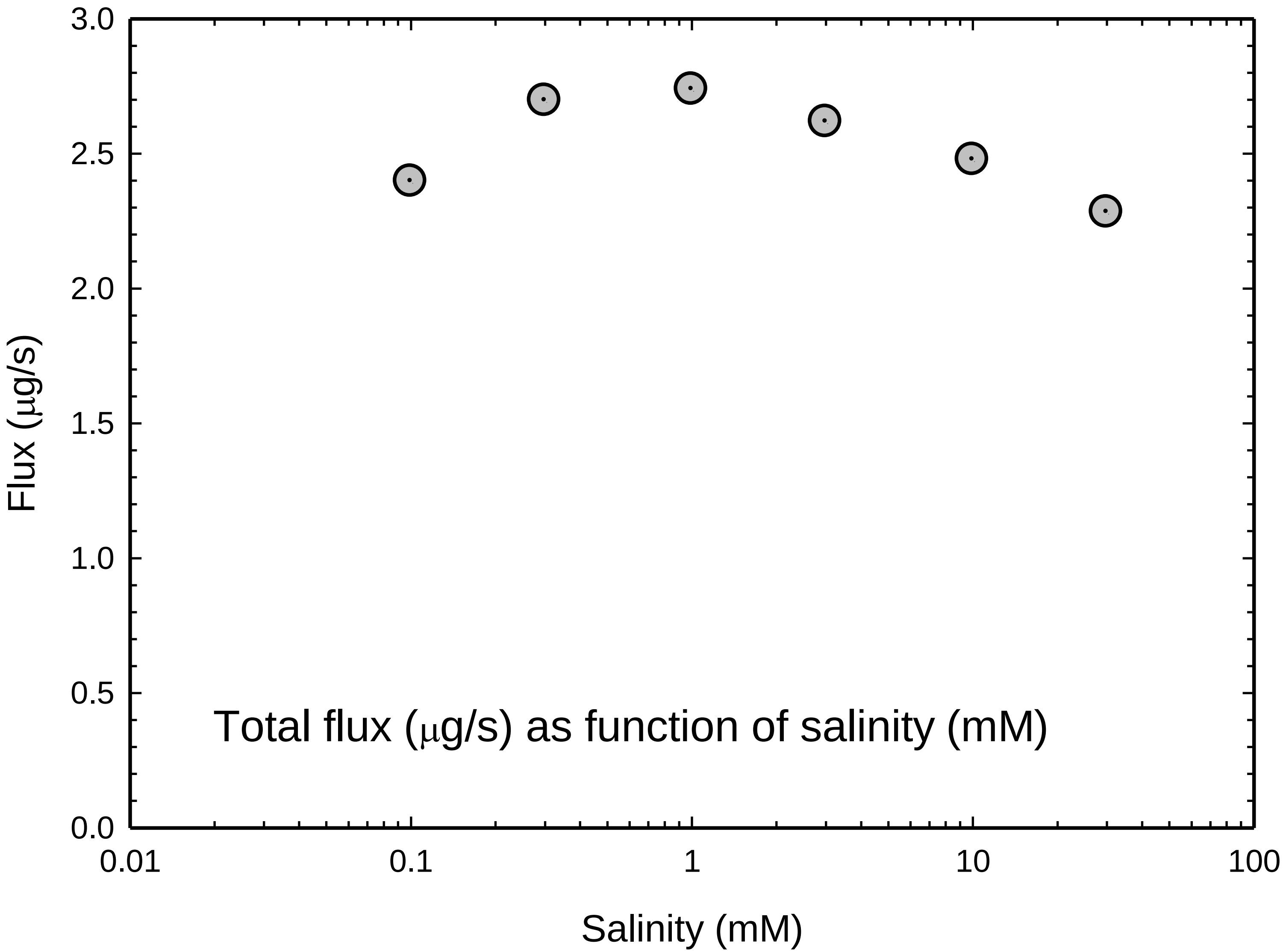
low limit for viscosity $$Q = 0.93 \times (vR)^{0.454}$$

higher limit $$Q = 0.74 \times (vR)^{0.305}$$





Results (2/2): r = 1 cm, flow velocity 6000m/a



Conclusions

Scaling estimates from the model obtained

- comparison to experiments?

The effect of different salinities in the models seems low

- swelling and erosion also with high salinities

Shape of the gel

- model does not match experiments

Steep gradient built in the model

- numerical difficulties in solving the model

Update on model development

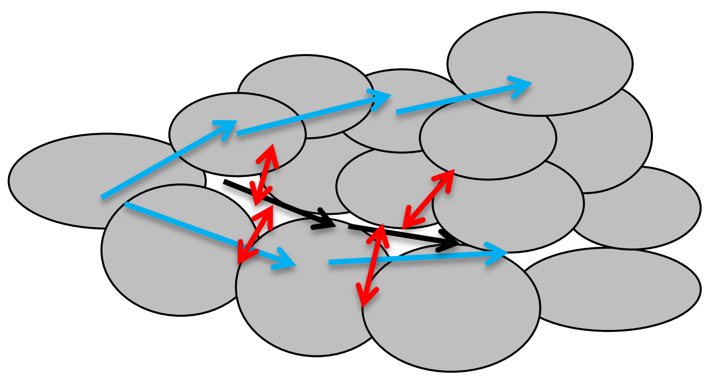
Objective

Objective is to build a model that includes the phenomena in slit erosion experiments

- swelling by wetting & salinity changes
- erosion mechanism
- solid → gel → sol → eroding particles and colloids carried away by the flow

Concept

- mechanical model – geometric frame for bentonite
  - same basic principles from solid to gel
- wetting by diffusion of “bound” water
- wetting by capillary action in “free porosity”
- transport of salt by moving water & diffusion
- salinity affects the “bound” water content
  - also role in breakdown mechanism



Energy considerations (1/6)

Let's first think of a sample of bentonite with a water mass content w in balance with water vapour of partial pressure p_p

Let's then increase the outer vapour partial pressure to $p_{p,out}$

- results in imbalance between the "bound" water and outer water potentials

unconfined sample

"$E_{free} = E_{out} - E_b^{uc}$"

confined sample

"$E_{free} = E_{out} - E_b^{c}$
$= E_{out} - (E_b^{uc} - E_{mech})$"

Energy considerations (2/6)

In terms of equations

Water vapour (and “bound” water) chemical potential

$$\mu = \mu_0 + RT\ \log\left(\frac{p}{p_0}\right)$$

Free energies

unconfined sample

$$E = \int_{n_0}^{n} \mu_{\text{out}} dn - \int_{n_0}^{n} \mu_{\text{b}}^{\text{uc}} dn$$

confined sample

$$E = \int_{n_0}^{n} \mu_{\text{out}} dn - \int_{n_0}^{n} \mu_{\text{b}}^{\text{c}} dn$$

$$= \int_{n_0}^{n} \mu_{\text{out}}\, dn - \left(\int_{n_0}^{n} \mu_{\text{b}}^{\text{uc}} dn - \int_{V} \int_{\varepsilon_0}^{\varepsilon} \boldsymbol{\sigma} : \mathbf{d}\boldsymbol{\varepsilon} dV \right)$$

Energy considerations (3/6)

The difference between unconfined and confined “bound” water chemical potentials has been observed to be equal to swelling pressure by e.g. ***Dueck and Börgesson***, ***Kahr et al.*** and ***Kassif and Shalom***

→ volume of the bentonite structure increases by the volume of “bound” water

→ “ bound” water is sorbed into the structure of bentonite

(integrated free energies should be used instead of potentials)

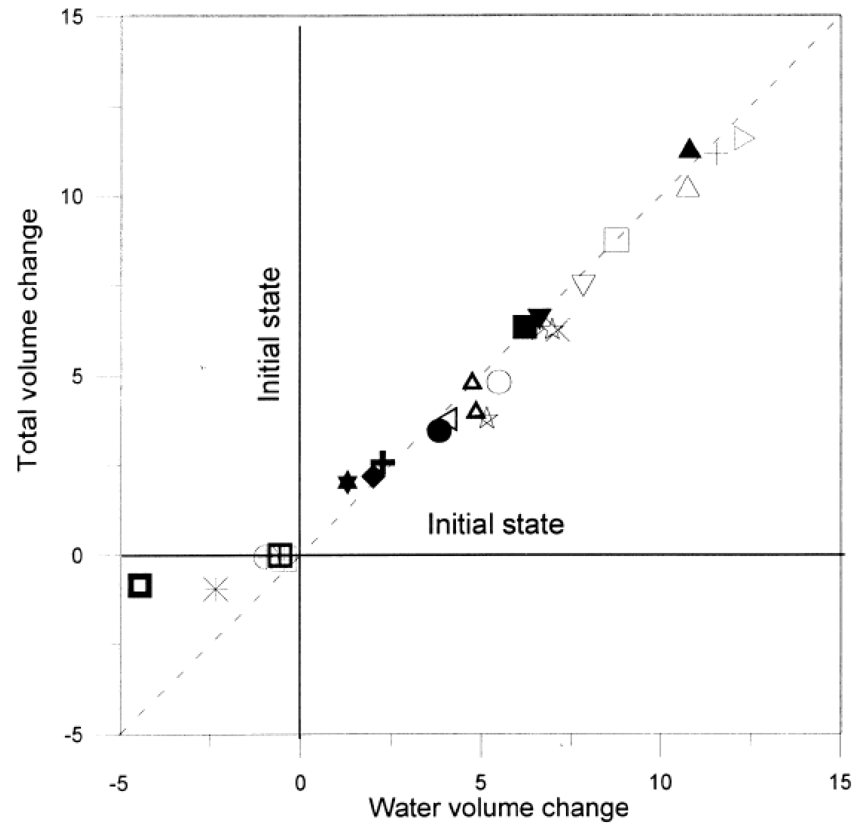
Dueck, A., Börgesson, L. (2007). Model suggested for an important part of the hydro-mechanical behaviour of a water unsaturated bentonite. Engineering Geology, 92, 160-169.
Kahr, G., Kraehenbuehl, F., Stoeckli, H.F., Müller-Vonmoos, M. (1990). Clay Minerals, 25, 499-506
Kassiff, G., Shalom, A. B. (1971). Experimental Relationshiop Between Swell Pressure and Suction. Géotechique, 21, 245-255.

Energy considerations (4/6)

Finding is supported by ***Cases et al. (1992, 1997)*** and ***Bérend et al.***

- water found to be adsorped mostly into interlayers

Direct observation by ***Delage et al.***



Provides coupling of the mechanical model from “bound” water content

Bérend, I., Cases, J. M., Francois, M., Uriot, J. P., Michot, L., Masion, A., Thomas, F. (1995). Mechanism of Adsorption and Desorption of Water Vapor by Homoionic Montmorillonites. 2. The Li^+, Na^+, K^+, Rb^+ and Cs^+-Exchanged Forms. Clays and Clay Minerals, 43, 324-336.
Cases, J. M., Bérend, I., Besson, G., Francois, M., Uriot, J. P., Thomas, F., Poirier, J. E. (1992). Mechanism of Adsorption and Desorption of Water Vapor by Homoionic Montmorillonite. 1. The Sodium-Echanged Form. Langmuir, 8, 2730-2739.
Cases, J. M., Bérend, I., Francois, M., Uriot, J. P., Michot, L., Thomas, F. (1997). Mechanism of Adsorption and Desorption of Water Vapor by Homoionic Montmorillonites. 3. The Mg^{2+}, Ca^{2+}, Sr^{2+}, Rb^+ and Ba^{2+} Exchanged Forms. Clays and Clay Minerals, 45, 8-22.
Delage, P., Howat, M.D., Cui, Y.J. (1998). The relationship between suction and swelling properties in a heavily compacted unsaturated clay. Engineering Geology, 50, 31-48.

Energy considerations (5/6)

diffusion of “bound” water is driven by the chemical potential gradient

- compare to Darcy’s law & van Genuchten eqs combination

$$\mathbf{j}_{\mathrm{m}} = \rho_{\mathrm{water}}\mathbf{v} = -\rho_{\mathrm{water}}\frac{D}{RT}\nabla\mu = -\rho_{\mathrm{water}}D\nabla\log\left(p_p(w)\right) = -\rho_{\mathrm{water}}D\frac{1}{p_p(w)}\nabla p_p(w) = -\frac{\rho_{\mathrm{water}}D}{p_p(w)}\frac{\partial p_p(w)}{\partial w}\nabla w$$

$$\mathbf{j} = \alpha\frac{\rho_{\mathrm{dry}}w}{\rho_{\mathrm{water}}}\mathbf{j}_{\mathrm{m}} = -\alpha\frac{\rho_{\mathrm{dry}}wD}{p_p(w)}\frac{\partial p_p(w)}{\partial w}\nabla w$$

$$\mathbf{j} = \alpha\frac{\rho_{\mathrm{dry}}w}{\rho_{\mathrm{water}}}\mathbf{j}_{\mathrm{m}} = -\left(\alpha\frac{\rho_{\mathrm{dry}}wD}{p_p(w)}\frac{\partial p_p(w)}{\partial w}\nabla w - k\nabla\left(\frac{1}{3}\mathrm{trace}(\boldsymbol{\sigma})\right)\right)$$

Energy considerations (6/6)

The salinity of water affects the outer chemical potential (compare to water vapour

"bound" water content dynamics: $R = kS_{\mathrm{free}}\left(\mu_{Na} - \mu_{\mathrm{pp}}^{\mathrm{c}}\right)$

potential of saline water > potential of bound water

→ more "bound" water → swelling

salinity may also change the mechanical parameters

Mechanical model

in generel elasto-viscoplastic

- elastic inside yield surface
  - two parameters, e.g. bulk *K* and shear modulus *G* needed
- yield surface
- plastic/viscous flow rule
- wall friction

from unsaturated solid to gel

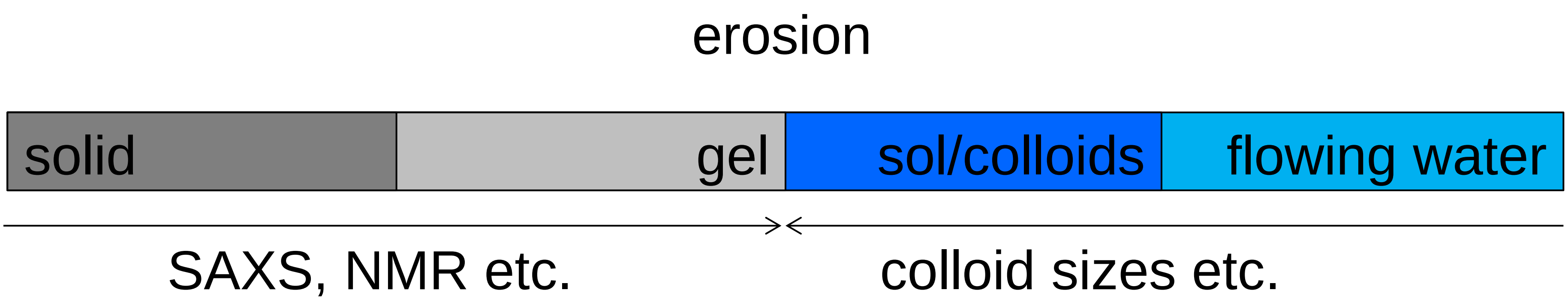
- gel parameters and model from TR-09-34 by ClayTech and BELBaR results by B+Tech
  - bulk modulus?
- parameters for unsaturated solid & stiff gel
  - ?
  - own experiments considered

Breakdown mechanism

Will be considered next

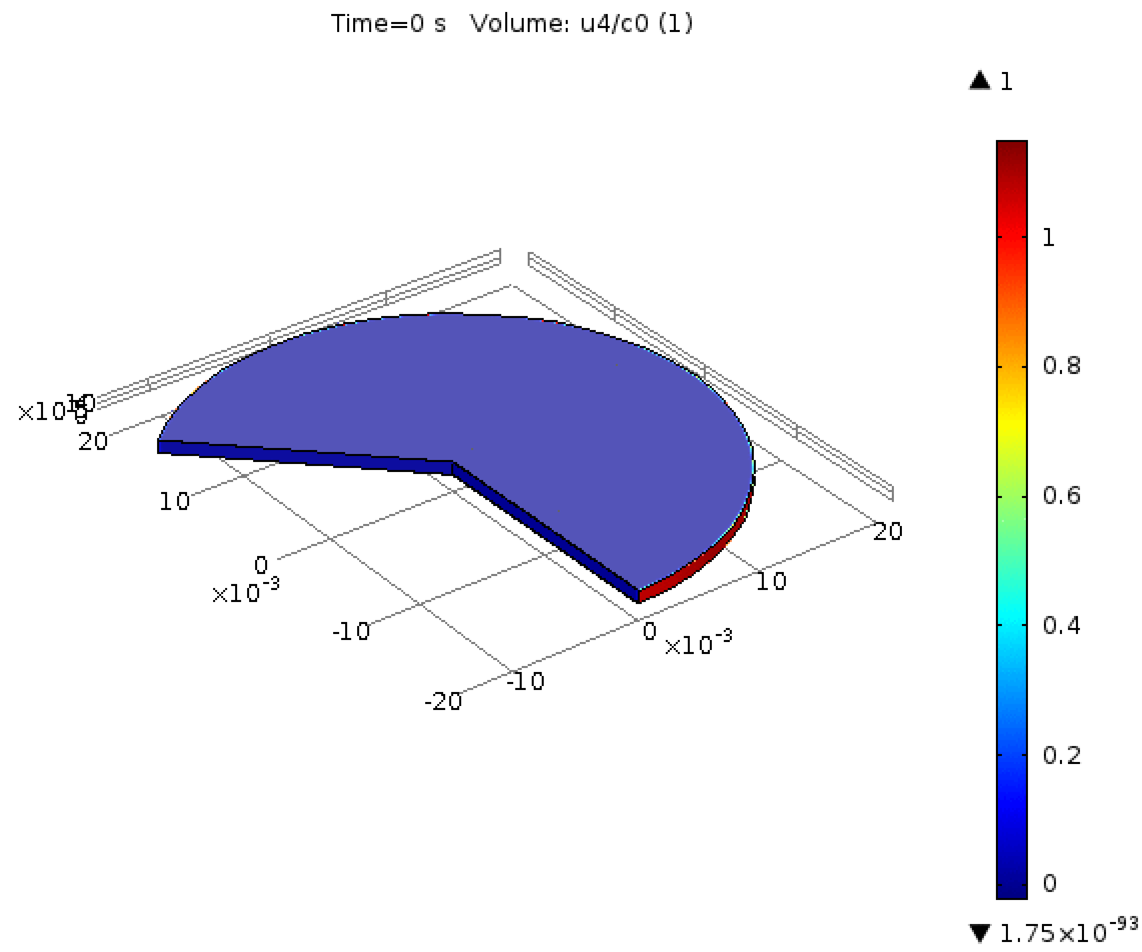
Simple: concentration of Na below CCC

More complicated: have to take a look at Grolimund’s presentation



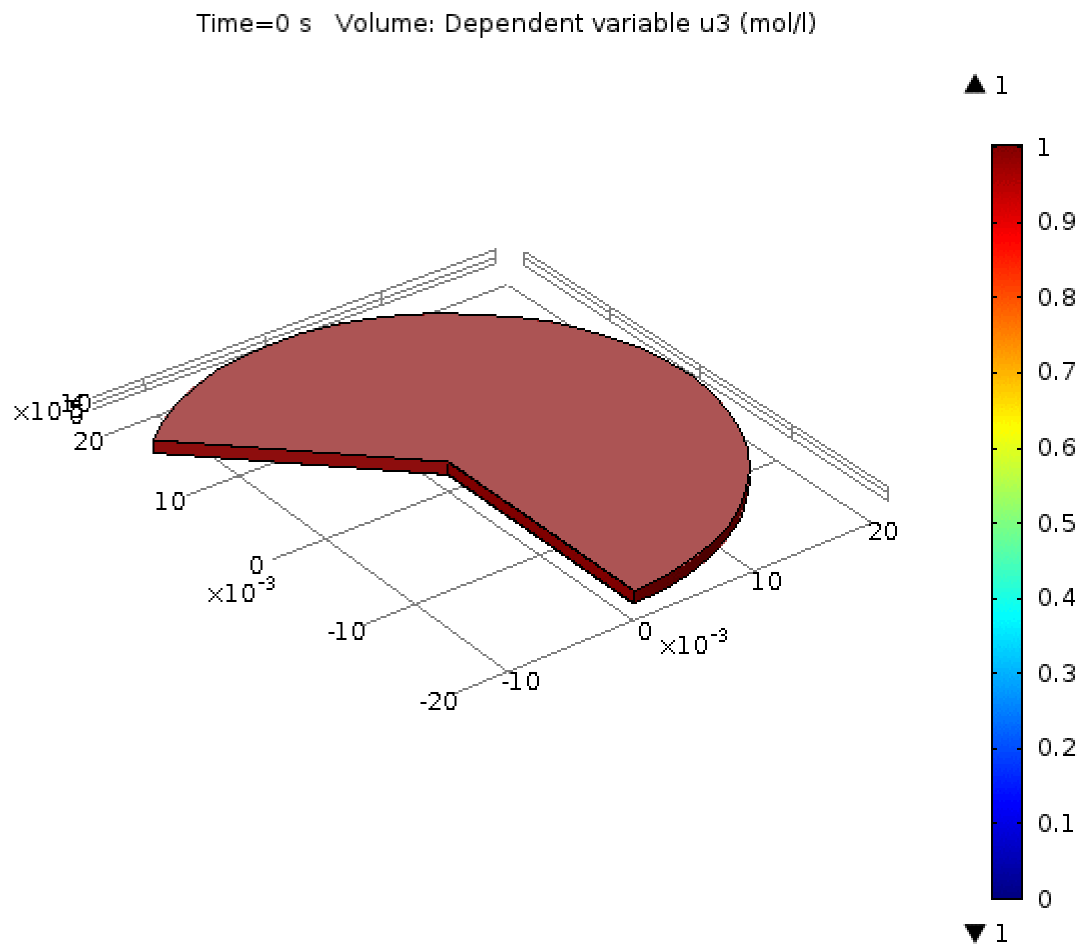
Swelling by wetting – an example

- water flow into bentonite in "free volume"
- NaCl in the free water
- diffusion of "bound" water
- coupling between salinity and "bound" water
- volume change of the structure by "bound" water
- parameters not realistic
- colour: saturation of "free" porosity



Swelling by lowering salinity – an example

- same as the earlier model + lowering salinity
- Na begins to diffuse out because of the connection to dilute water
- lowering salinity increases the amount of “bound” water
- volume change of the structure by the “bound” water amount increase
- parameters not realistic
- colour: salinity



Summary

A model framework established

- mechanical model
- diffusion of “bound” water
- diffusion of salt
- movement of “free” water when wetting

Couplings

- “bound” water increase by wetting or by lowering salinity
- volume change of structure by “bound” water
- lowering diffusion potential by swelling stress

Next steps

Model still under development

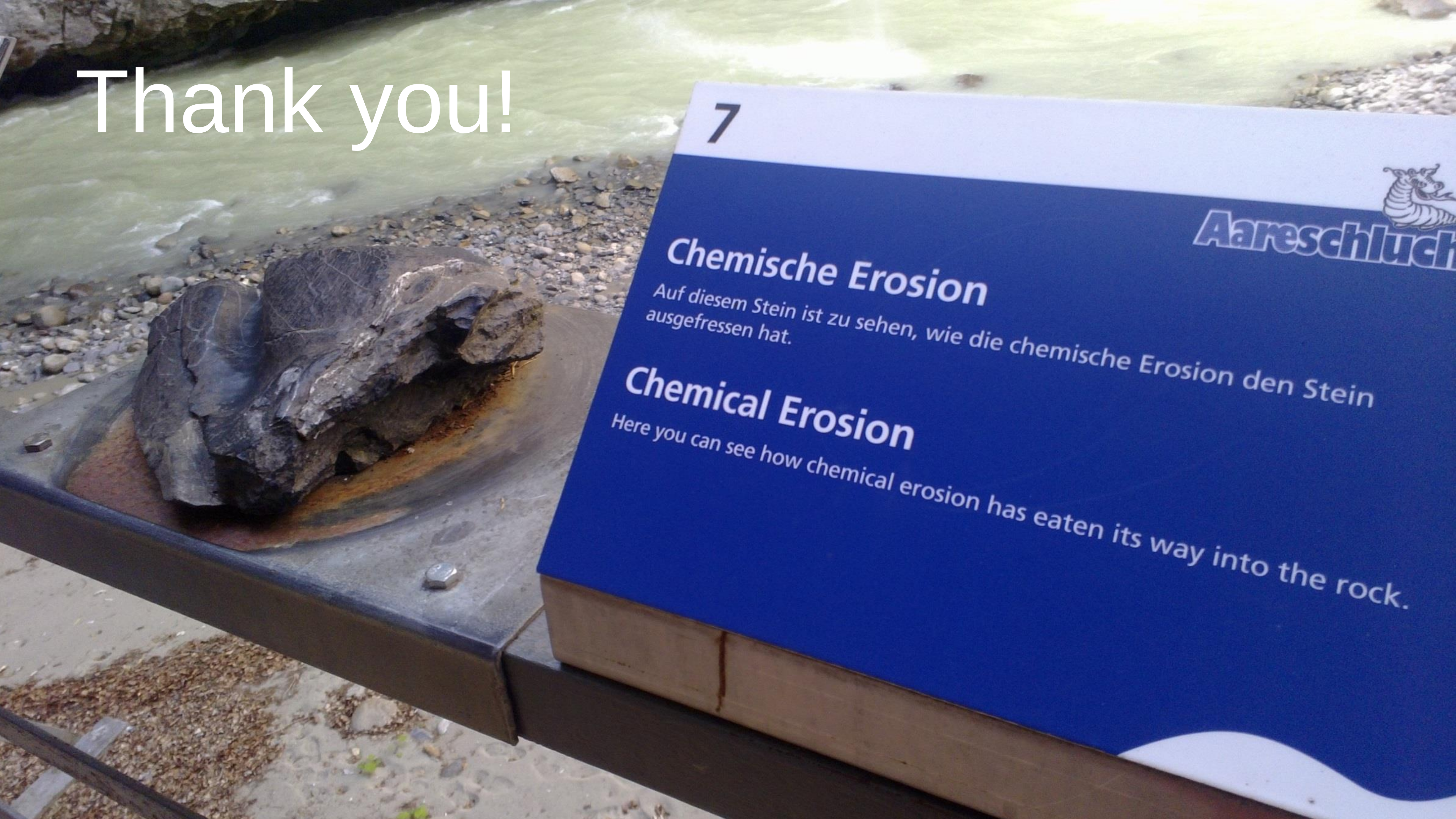
Breakdown mechanism

Details right

Implementation right

Real material parameters

Thank you!



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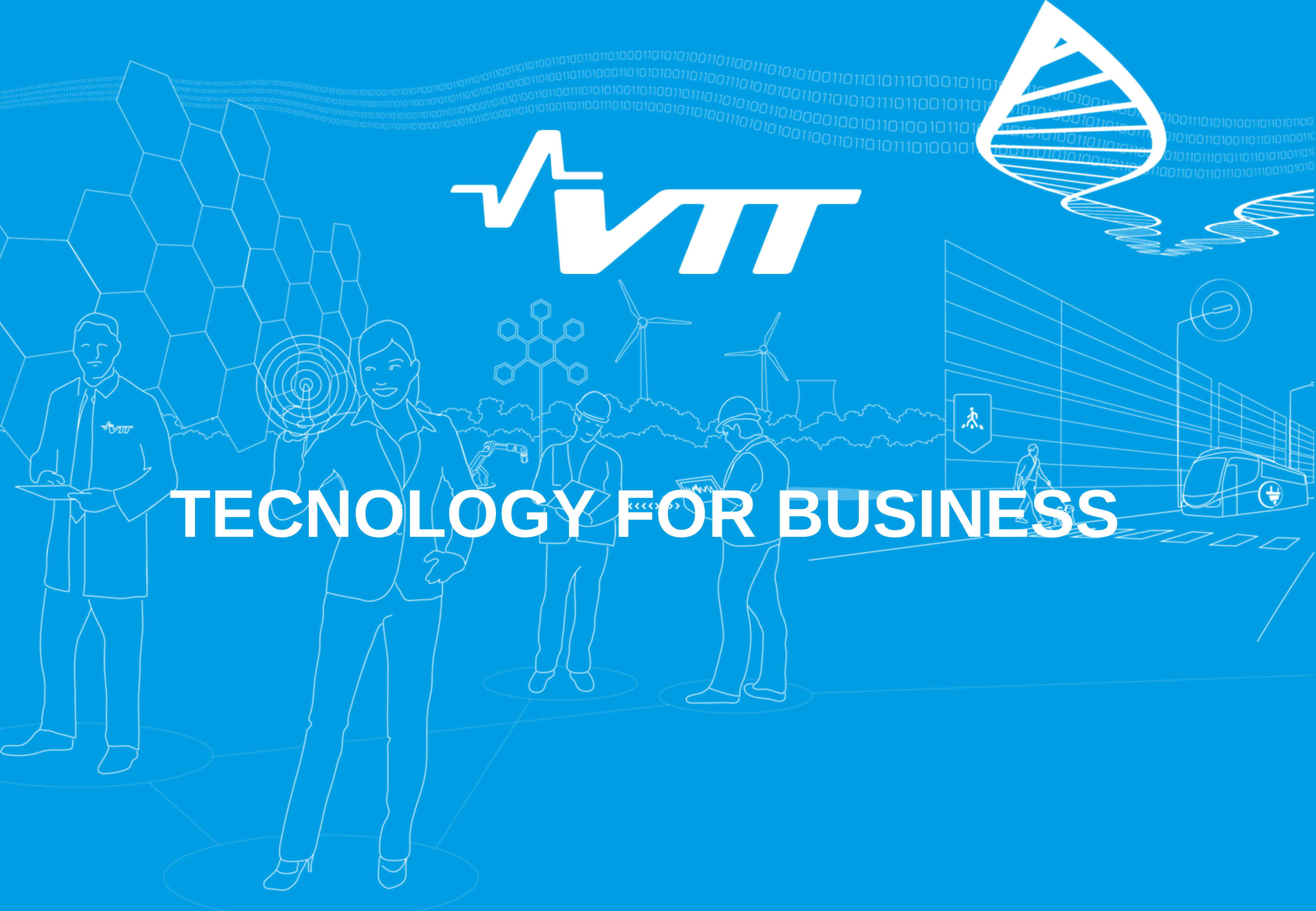
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