Faculty of Geosciences
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Molecular dynamics simulations of diffusive properties of stressed water films in quartz and clay grain contacts

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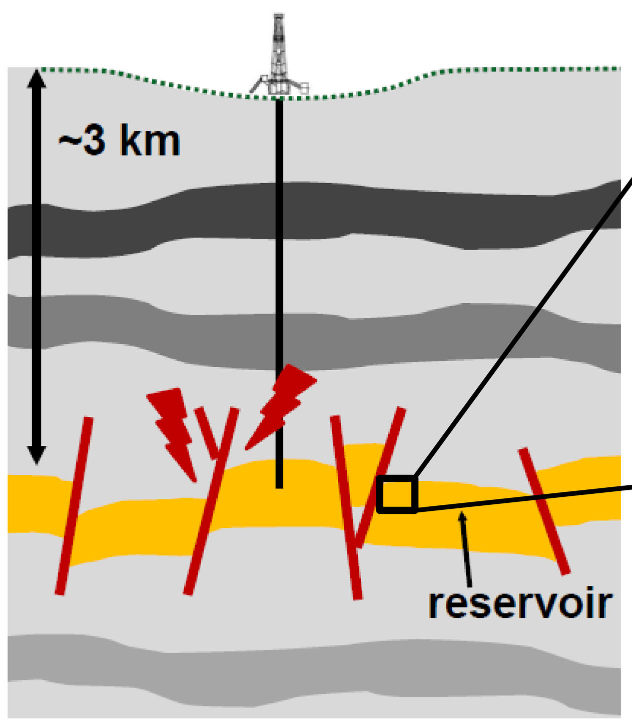
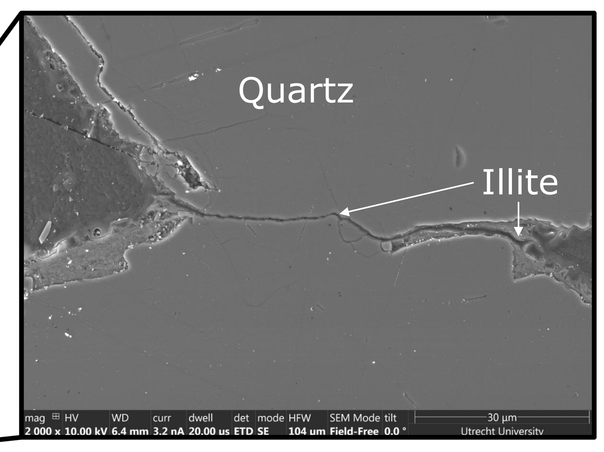
Introduction

Hydrocarbon production can increase effective normal stresses in reservoirs, inducing deformation and seismicity[1]. The kinetics of time-dependent inelastic processes as pressure solution, that could persist long after production, are badly constrained. These processes can be limited by diffusive transport, which depends strongly on the product of fluid film thickness (d) and the diffusivity (D) at stressed grain contacts[2].

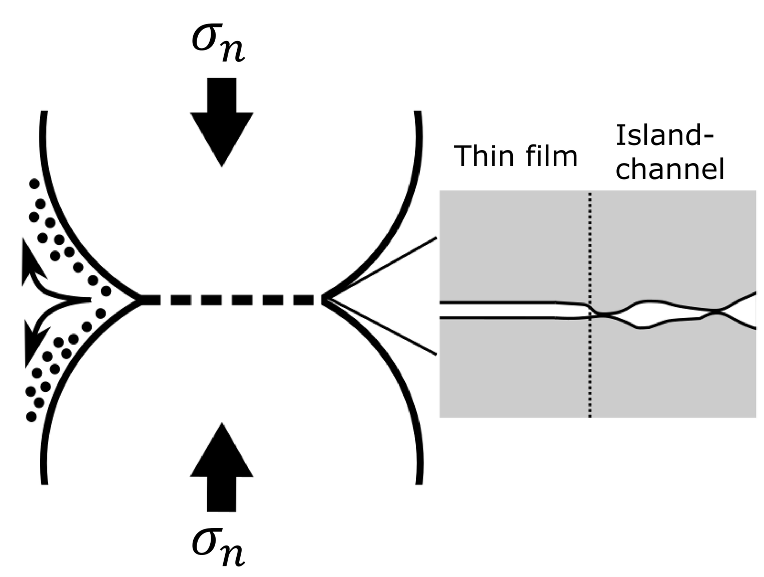
To predict the long-term response of reservoirs d·D must be quantified, but this is difficult to achieve in an experiment. Therefore, we perform molecular dynamics simulations with the parallel code LAMMPS to model stressed fluid film behaviour. Here we present the preliminary results on a grain contact with 10-10 quartz surfaces and water as a fluid under reservoir conditions.

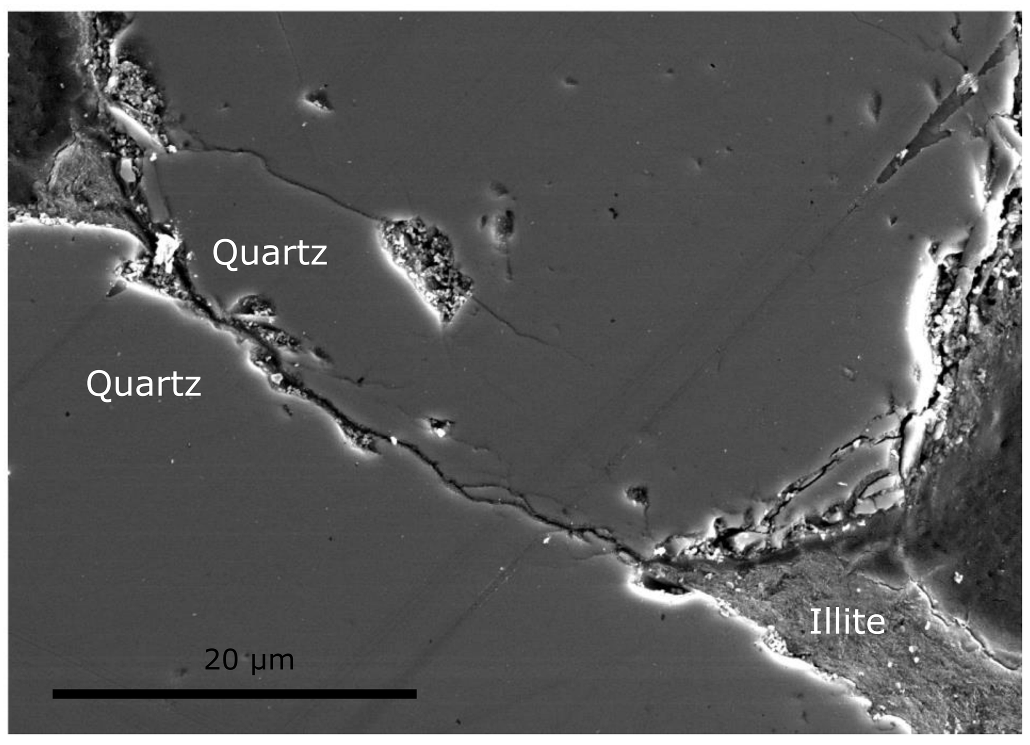


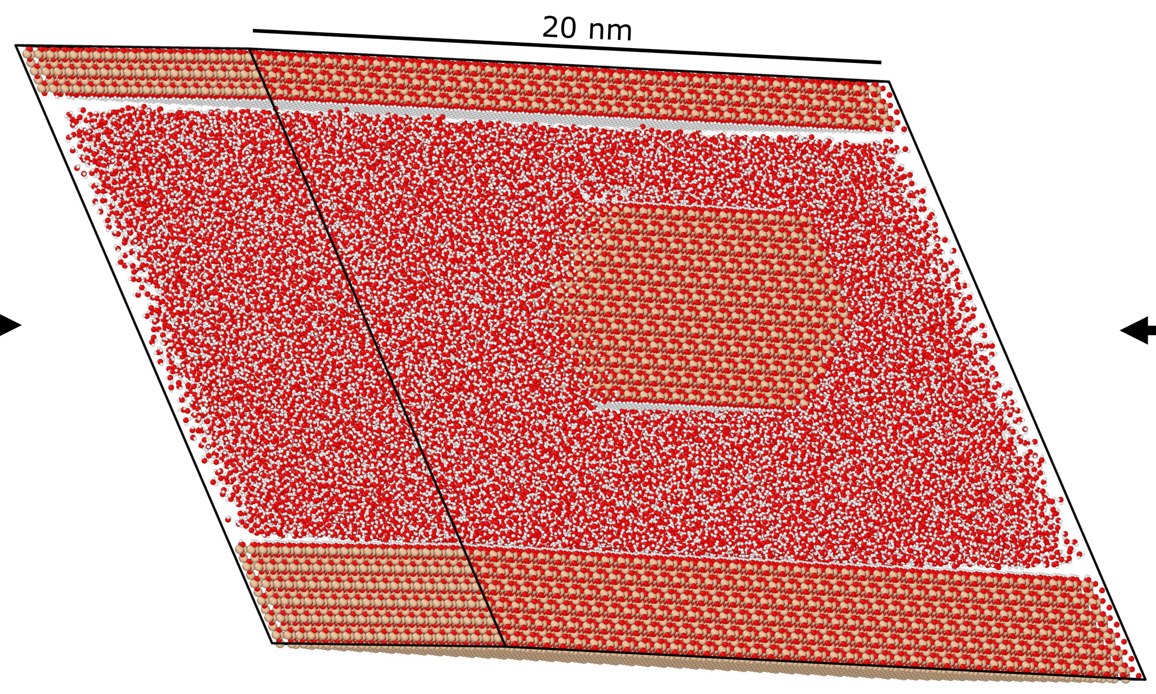


$$\dot{\varepsilon} = K_{eff} \cdot \Delta\mu_{Qtz\ contact-pore}$$

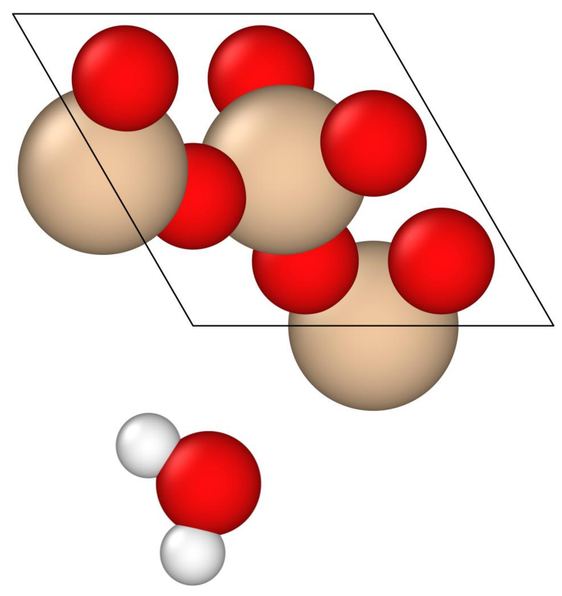
$$K_{eff} = \frac{8\boldsymbol{Dd}}{a^2 l^{eq}} \rho^f C_0^{eq} \frac{V_m}{RT}$$





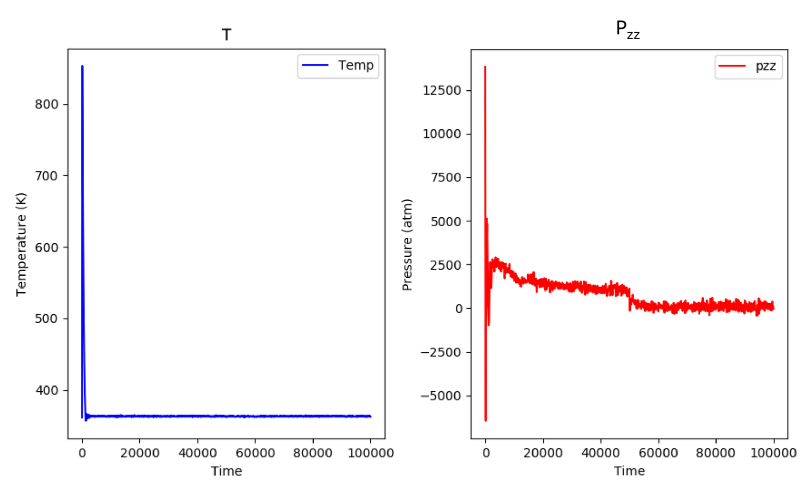


+ Hydroxylation



Equilibrate to T = 373K and P_f = 8 MPa

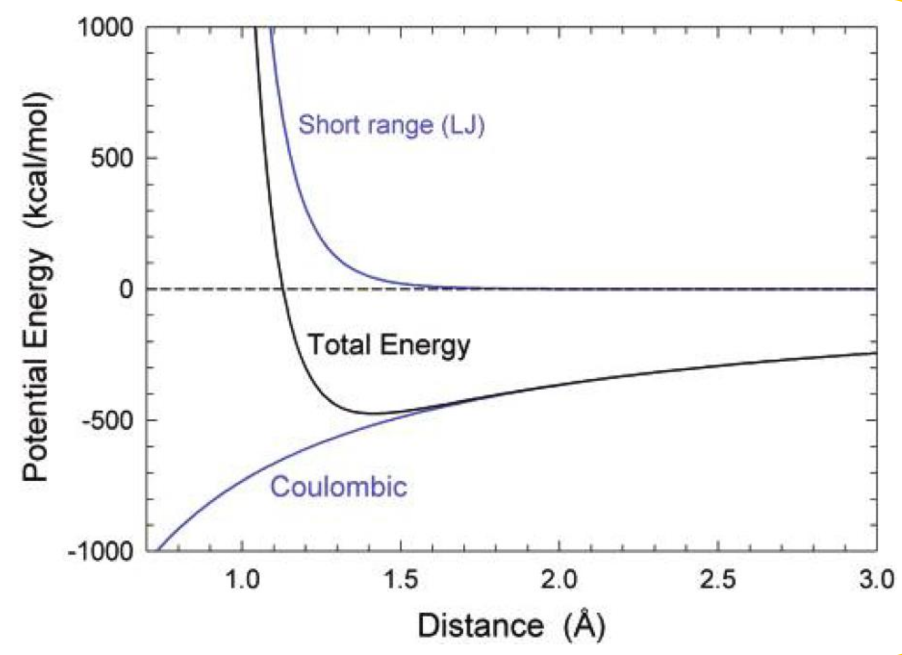
Nose-Hoover thermostat and barostat:
1. NVT ensemble
2. NPT ensemble



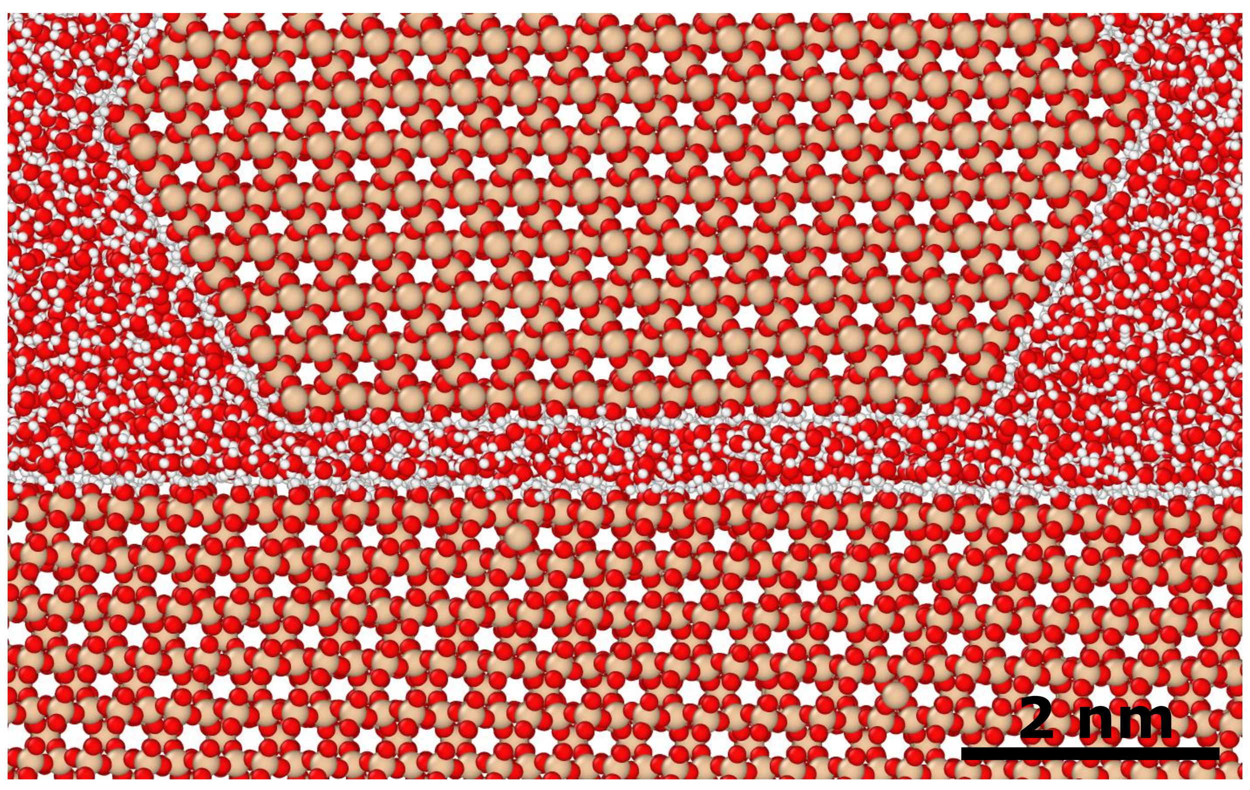
Solving Newton's equations of motion

ClayFF Force Field[3]

- Lennard-Jones potential
- Coulombic interactions
- Explicit bond stretch and angle terms for hydroxyl groups and water molecules (SPC)



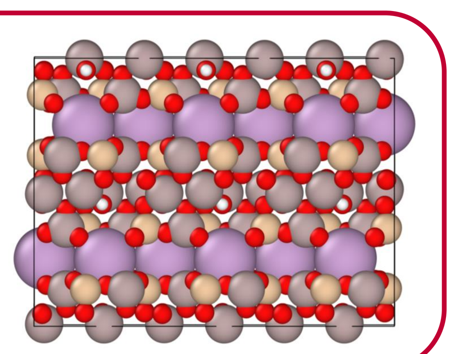
Apply σ_n^{eff} = 100 MPa to the contact



Diffusion Coefficient: Einstein relation

$$MSD = \langle |\boldsymbol{x}(t) - \boldsymbol{x}_o|^2 \rangle \qquad D = \frac{1}{2n} \lim_{\tau \to \infty} \frac{dMSD(\tau)}{d\tau}$$

Illite



Conclusions

The stressed fluid films in our simulations reach steady-state thicknesses after run times on the order of nanoseconds. Under reservoir conditions, the thicknesses are reduced to less than a nanometer, but multiple adsorbed layers of water remain.

Next steps

We will perform production runs on the Dutch national supercomputer Cartesius for statistically significant calculations of film thickness and mean square displacement (MSD). With these data we can explore the chemical implications of the changing water structure in the stressed fluid film. This will then be expanded to quartz-clay systems.

References

1. Pijnenburg, et al. (2019). Journal of Geophysical Research: Solid Earth
2. Lehner, F. K. (1995). *Tectonophysics*, *245*(3-4), 153-170.
3. Cygan et al. (2004). The Journal of Physical Chemistry B, 108(4), 1255-1266.