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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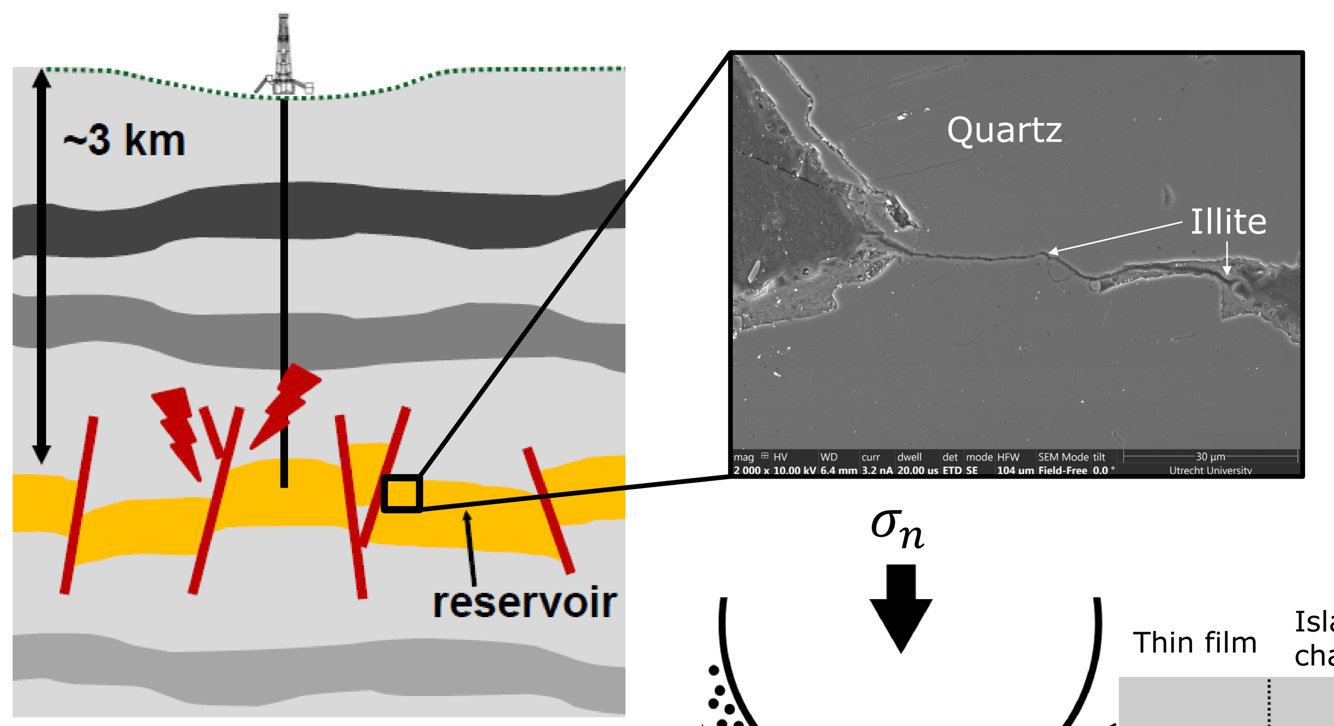
Introduction

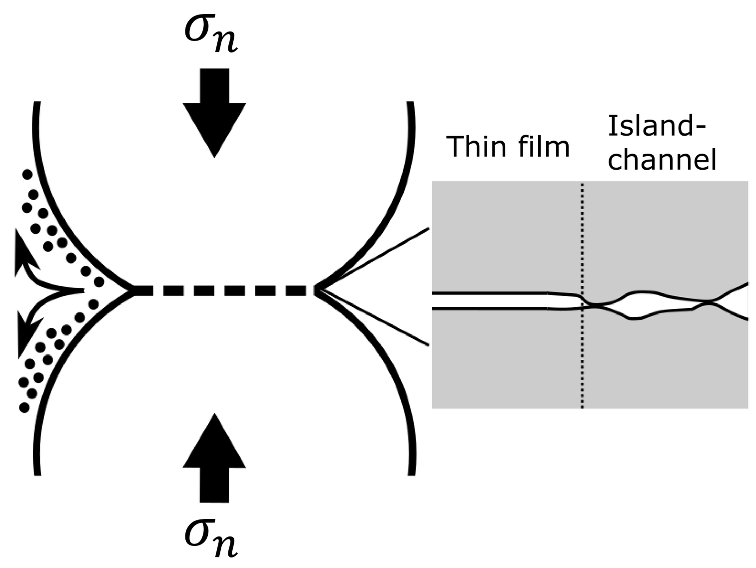
Hydrocarbon production can increase **effective normal stresses** in reservoirs, inducing **deformation** and seismicity[1]. The kinetics of **time-dependent** inelastic processes as **pressure solution**, that could persist long after production, are badly constrained. These processes can be limited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

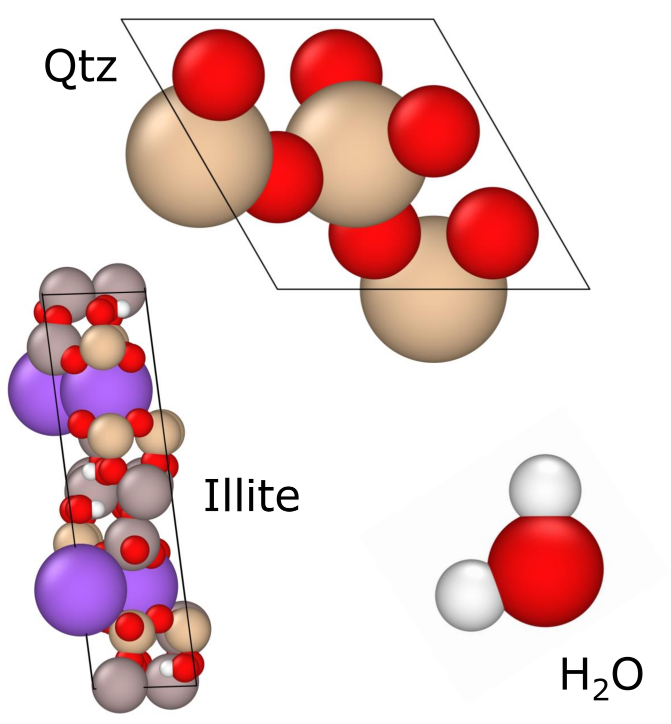
To predict the long-term response of reservoirs d·D must be quantified, but this is difficult to achieve in an experiment. We perform **molecular dynamics** simulations with the parallel code LAMMPS to model stressed and confined fluid film behaviour. Here we present preliminary results of a contact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



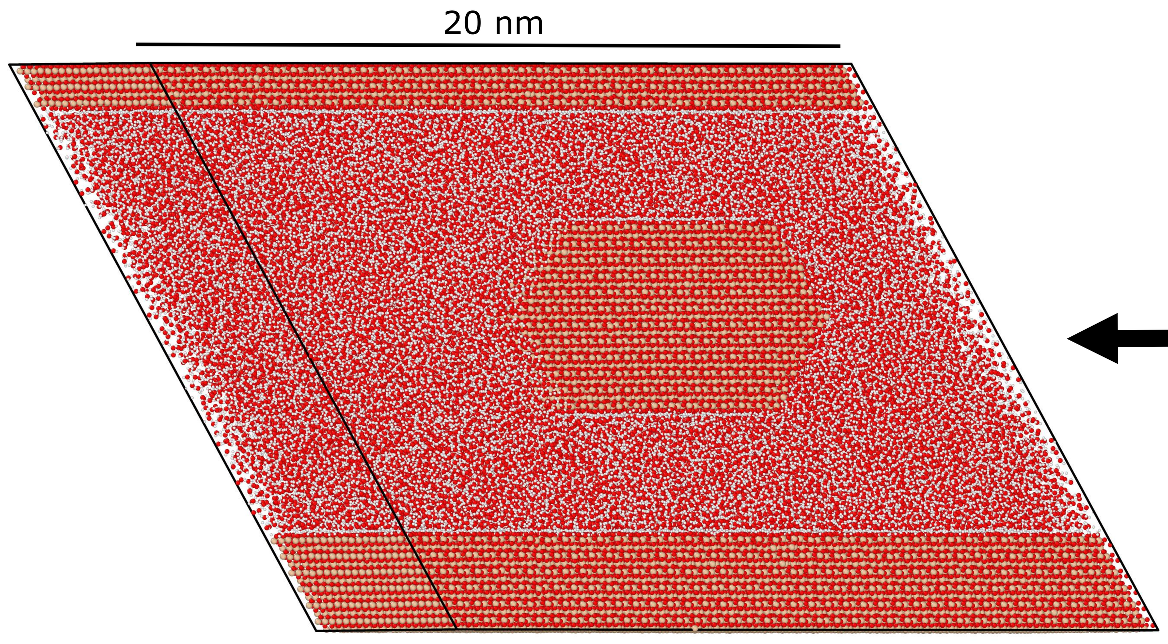
$$\dot{\varepsilon} = K_{eff} \cdot \Delta\mu_{Qtz\ contact-pore}$$

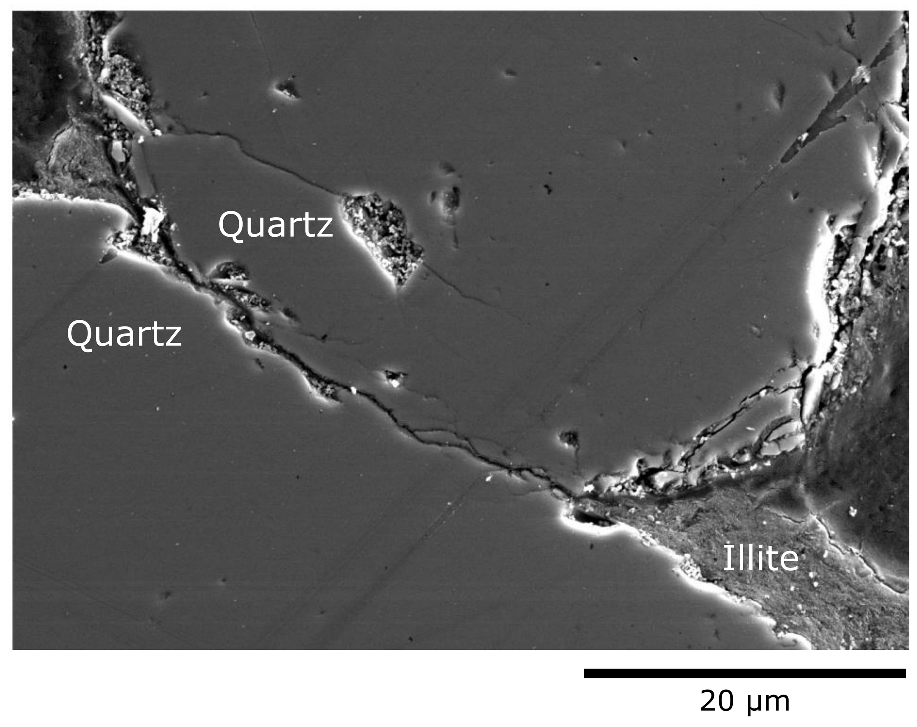
$$K_{eff} = \frac{8Dd}{a^2 l^{eq}} \rho^f C_0^{eq} \frac{V_m}{RT}$$

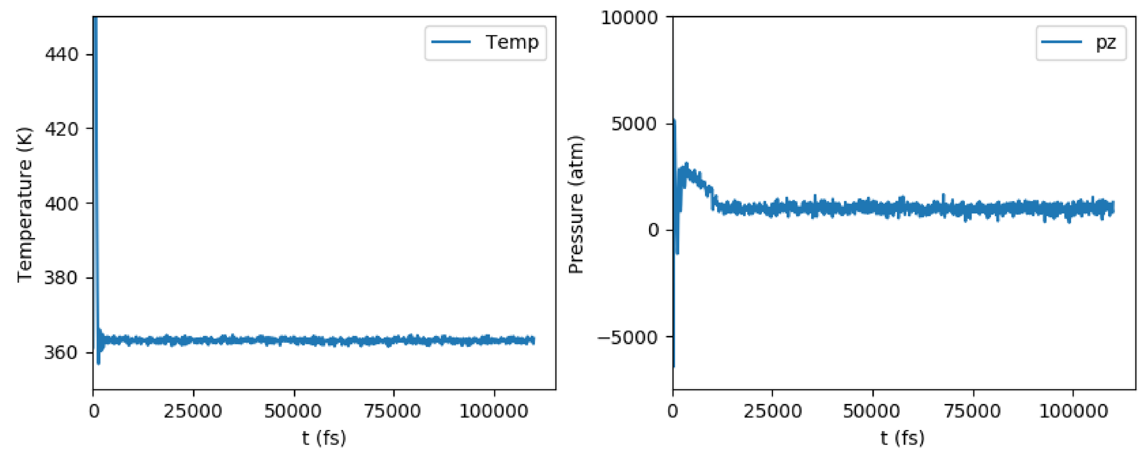




Hydroxylation



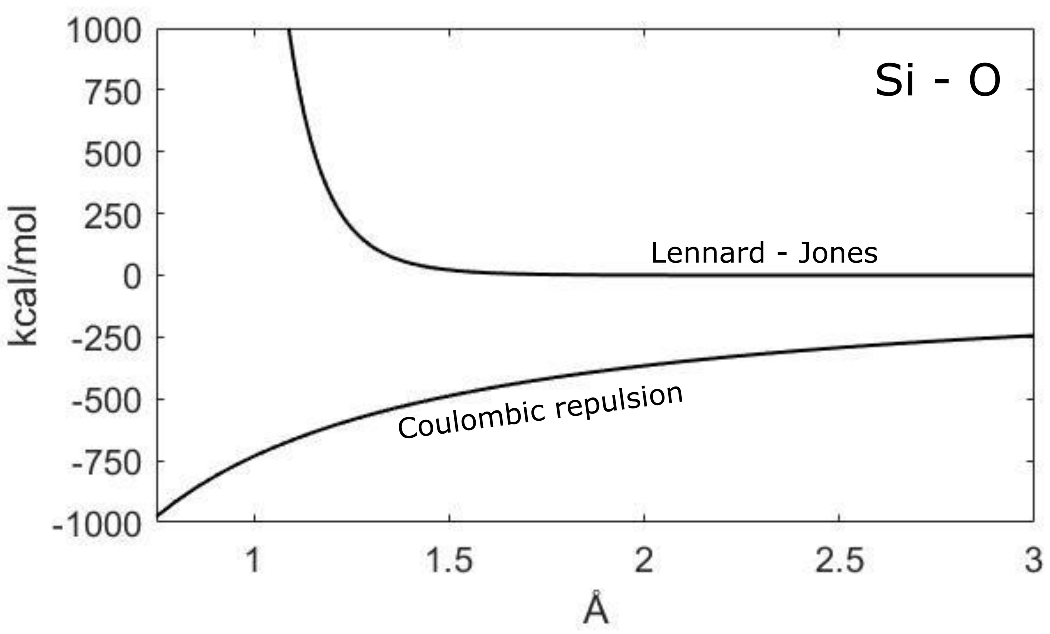




Equilibrate to T = 373K and P_f = 8 MPa with Nosé-Hoover thermostat and barostat

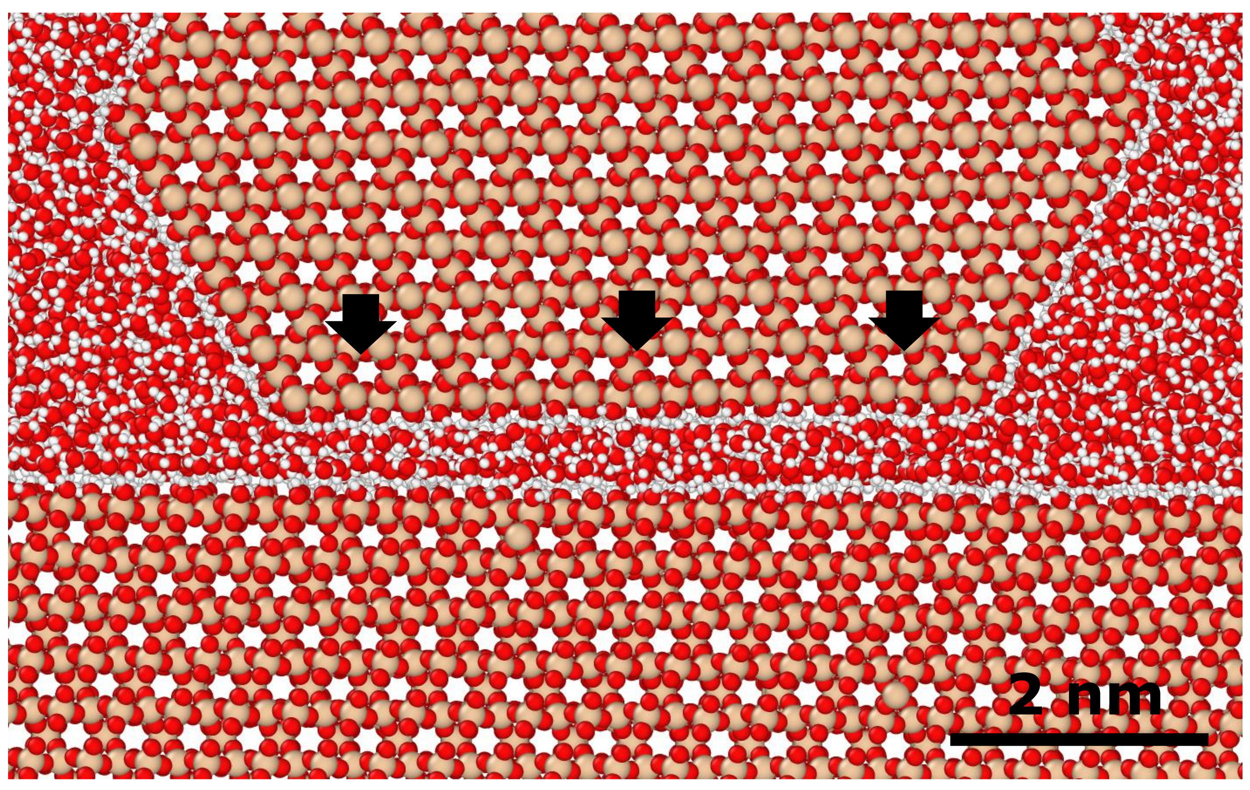
Add interatomic potentials

- ClayFF Force Field[3]
- Lennard-Jones (VDW) potential
- Coulombic interactions
- Flexible SPC[3] water model with explicit bond terms



Solving Newton's equations of motion

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



Find *D* coeff. For the eq. thickness *d*

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 the confined fluid's diffusivity. With these data we can explore the chemical implications of the changing water structure in the stressed fluid film. This set-up will then be expanded to the range of conditions and geometries found in reservoir sandstones

Diffusion Coefficient

Einstein relation: $\langle \Delta \boldsymbol{r}^2 \rangle_t = \left\langle \left| \boldsymbol{r}_{i,t} - \boldsymbol{r}_{i,o} \right|^2 \right\rangle$ $\qquad D = \frac{1}{2n} \frac{\langle \Delta \boldsymbol{r}^2 \rangle_t}{t}$

Green-Kubo: $vacf(t) = \langle \boldsymbol{v}(t')\, \boldsymbol{v}(t'+t) \rangle$ $\qquad D = \int_{-\infty}^{\infty} vacf(t)\, dt$

References

1. Pijnenburg, et al. (2019). Journal of Geophysical Research: Solid Earth
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3. Cygan et al. (2004). The Journal of Physical Chemistry B, 108(4), 1255-1266.