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

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Hydrocarbon extraction can increase effective normal stresses in geological reservoirs, potentially inducing deformation and seismicity¹. The kinetics of time-dependent creep processes that could persist long after production has ended, such as pressure solution and stress corrosion, are poorly quantified. These processes can be limited by diffusion efficiency at stressed grain contacts, which depends strongly on fluid film thickness as well as interfacial and surface energies. The diffusive properties of stressed fluid films between various crystallographic surfaces of the rock forming minerals clay and quartz are critical to predict long term deformation of reservoir. Due to the small length scales of grain contacts, experimental data on these quantities are difficult to acquire. Therefore, we use molecular dynamic simulations to elucidate the physico-chemical behaviour of fluid films at different mineral interfaces.

We apply large-scale classical molecular dynamics in LAMMPS to numerically resolve fluid film behaviour in grain contacts. The silicate-water system is modelled using a modified ClayFF force field². A β-quartz block was placed within a water-filled nanopore with either hydroxylated β-quartz or basal illite clay surfaces as walls. This geometry was built using the software packages Atomic Simulation Environment, Ovito and Packmol. The system was first equilibrated using an NVT thermostat and an NPT barostat for tens of picoseconds under conditions of 8 MPa fluid pressure and a temperature of 100°C. Then, a force was applied on the quartz block, corresponding to 10-200 MPa normal contact stress, such that a thin water film is squeezed at the interface between two grains. Self-diffusion constants were calculated by mean square displacements and velocity autocorrelation in films at steady state thicknesses.

Simulations reach a steady state after several nanoseconds run time. Under reservoir conditions, fluid film thicknesses are reduced to less than one nanometre. Two to three layers of adsorbed water remain in the grain contact, a result consistent with reported fluid film properties for grain
contacts in upper crustal systems. Our results quantify how various juxtaposed quartz surfaces and quartz-clay interfaces influence fluid film thickness, self-diffusion and the dynamics of the water layer, which allows for constraining the kinetics of pressure solution creep in sandstone reservoirs.

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