# MD Simulations of Low-Salinity Enhanced Oil Recovery

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The aim of this research is to bring clarity to the fundamental mechanisms of clay-oil-brine interfaces that underpin low-salinity enhanced oil recovery (EOR), a technique whereby sea water, partially desalinated, is used to push increasing amounts of crude oil from existing, and future, oil reservoirs, increasing the reservoir lifetime and overall production.

Using large-scale molecular dynamic (MD) simulations to model the interactions of several different clays (montmorillonite, kaolinite and illite) interacting with various model oil compounds, we have been able to analyze the phenomena of low-salinity EOR at the molecular level, Figure 1.

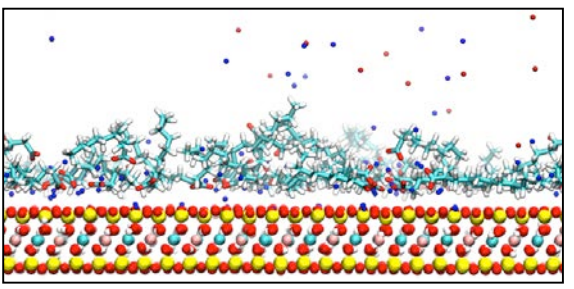

*Figure 1:* ***A snapshot presenting the interaction between an oil-wet montmorillonite clay particle and charged decanoate molecules.***

Our work presents an increasingly high-resolution picture of low-salinity EOR, whereby it is observed that the effects of double layer expansion cannot explain the phenomenon of low-salinity enhanced oil recovery. Rather, the results show that it is the pH level surrounding the clay in conjunction with the presence of divalent cations that is the determining factor driving the titular effect [1, 2].

[1] Underwood, Erastova, Cubillas & Greenwell (2015), *J Phys. Chem. C* **119.13**, 7282-7294. [2] Underwood, Erastova & Greenwell (2016); *J. Phys. Chem. C* **(Submitted)**