Applying Molecular Dynamics Simulations in the Context of Enhanced Oil Recovery

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40% of oil cannot be extracted from an oil well due to its strong physical interactions with the rock walls. This project aims to explain the interactions using molecular dynamic simulations and first-principle calculations to increase oil wells' yield. Existing crude oil models consider only a few components that make predictions less accurate. Also, their large size prevents simulating them with other materials, such as saline water and organic solvents, to study their wettability alteration. The purpose of this project is to overcome the size issue by using a smaller and more comprehensive model to simulate the interactions of most of the major components in crude oil with the most abundant rock, calcite. Using GROMACS in the Shaheen Supercomputer, the interaction of over 13,000 atoms was simulated to test the smaller model. Simulation results showed the organic molecules form five distinct adsorption layers that are parallel to the (104) calcite surface. Such an alignment makes the interaction between the rock and oil stronger. The results matched previous larger models. Also observed were that some gas molecules, such as carbon dioxide, can penetrate through the layers and interact with the calcite surface directly. Saline water of different compositions and organic solvents can make the interaction weaker, pointing out a good potential of using them to find a cost-effective wettability altering material. These findings show a promising future for enhanced oil recovery that will further increase the amount recovered from a single well.