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Quarterly Report

Understanding Multicomponent Multiphase Hydrocarbon Fluid Interaction and Transport in Shale Matrix: From Nanoscale to Wellbore Production

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WORK PERFORMED UNDER

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1.0 GOALS OF PROJECT

One critical issue related to shale oil/gas production is a rapid decline in wellbore production and a low recovery rate. Therefore, maximizing wellbore production and extending the production life cycle are crucial for the sustainability of shale oil/gas production. Shale oil/gas production starts with creating a fracture network by injecting a pressurized fluid in a wellbore. The induced fractures are then held open by proppant particles. During production, oil and gas release from the shale matrix, migrate to nearby fractures, and ultimately reach a production wellbore. Given the relatively high permeability of the induced fractures, oil/gas release and transport in low-permeability shale matrix are likely a limiting step for long-term wellbore production. This project is aimed to (1) fundamentally understand the disposition and release of complex hydrocarbon mixtures in nanopore networks of shale matrix and their transport from low-permeability matrix to hydrofracking-induced fractures under various reservoir conditions ranging from black oil to dry gas and (2) use machine learning to upscale and integrate the nanometer-scale understanding into reservoir-scale model simulations. The work will help develop new stimulation strategies to enable efficient resource recovery from fewer and less environmentally impactful wells.

2.0 ACCOMPLISHMENTS

Molecular dynamics (MD) simulations on oil flow enhancement in shale nanopores: MD simulations were performed to study the multicomponent interaction of octane, supercritical CO_2 ($scCO_2$), H_2O in inorganic (muscovite) and organic (kerogen) nanopores. The study focused on the effect of adding CO_2 and/or H_2O into nanopores on the friction and viscosity of octane with pore surface, and on the role of friction and viscosity in the flow enhancement. The analysis will provide a molecular origin on the flow enhancement when adding additives into the system. Two porous materials were selected for study: (1) inorganic media represented by muscovite (i.e. denoted as M) and (2) organic materials modeled by kerogen (denoted as K). Different pore fluids including octane (i.e., denoted as O), water (H_2O), and carbon dioxide (CO_2) were placed in a muscovite or kerogen nanopore. For example, in the M_O_CO_2_H_2O system, octane, CO_2, and H_2O coexist in the muscovite nanopore. In the K_O_H_2O system, both octane and H_2O are present in the kerogen nanopore. Simulation snapshots are shown in Figure 1.

The results indicate that in the inorganic nanopore, both water and CO_2 enhance the flow rate of octane. Water significantly reduce the friction coefficient of octane with inorganic surface, while CO_2 significantly reduce both friction coefficient and viscosity of octane. In the organic nanopore, water play little role in the enhancement of flow rate. CO_2 reduce the friction coefficient of octane with kerogen surface and reduce the viscosity of octane. These results indicate that CO_2 can be used as an oil enhanced recovery factors that works for both inorganic and organic pores in shale reservoirs. H_2O on the other hand just works for the inorganic nanopores.

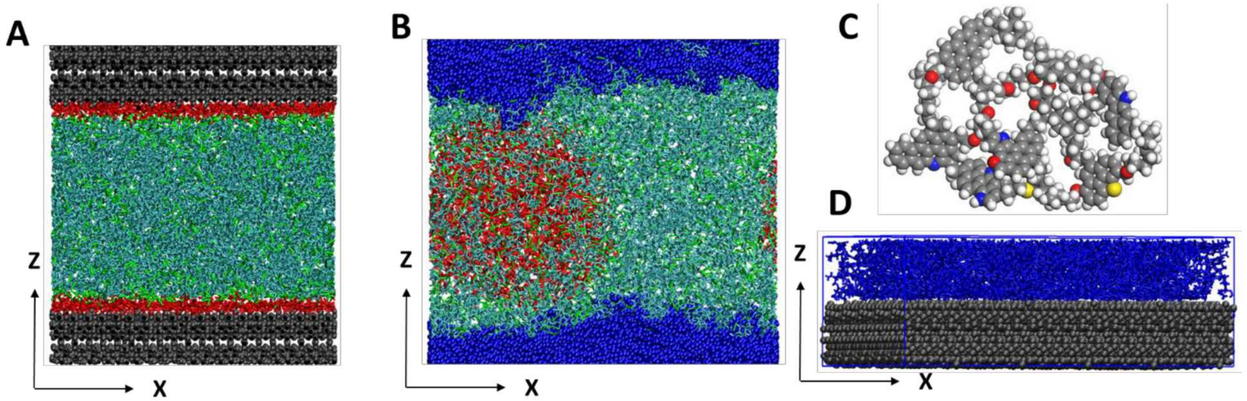

Figure 1. Simulation snapshots demonstrates water (red), CO_2 (green), and octane (cyan) confined in muscovite (gray) (A) and kerogen (blue) (B) nanopore. Molecular structure of immature kerogen found in the shale oil reservoir (C). Silver, white, red, blue, and yellow spheres represent carbon, hydrogen, oxygen, nitrogen, and sulfur atoms, respectively. Simulation snapshot illustrates the kerogen and muscovite system used to construct the kerogen surface (D).

Interaction of kerogen with brine saturated supercritical CO_2: Injection of supercritical CO_2 into a subsurface geologic formation has been considered as a possible means for mitigating anthropogenic carbon emission. Supercritical CO_2 has also been proposed as a stimulating agent for enhanced hydrocarbon recovery in unconventional reservoirs with a possibility for simultaneous carbon sequestration. As a key component of shale formations, kerogen and its interaction with injected CO_2 will directly determine the capacity and caprock integrity of a carbon storage system as well as the potential for hydrocarbon recovery in an unconventional reservoir. A mechanistic understanding of this interaction yet needs to be developed. In this work, a set of experiments on kerogen interaction with brine-saturated supercritical CO_2 under relevant reservoir conditions (90 °C and 2800 psi pressure) were performed. Over up to 30 days of reaction time, the reaction of kerogen with brine-saturated supercritical CO_2 was surprisingly extensive (Figure 2). The reaction is highly selective and heterogenous. Some grains were completely reacted and turned into char whereas others were only sporadically reacted. The reaction led to significant losses of carbon, hydrogen, sulfur and nitrogen contents and removal of aliphatic, aromatic and carboxyl function groups. The atomic ratio of lost hydrogen to carbon was determined to be 3.26; however, the oxygen content increased, which is apparently distinct from a regular thermal maturation process whereby both hydrogen and oxygen contents generally decrease. Also, the reaction removed more than 50% of original pyrolysable carbon, which was either converted into char or dissolved into brine solution. The char accounts for 12% of total carbon in reacted kerogen.

The reacted kerogens, despite their smaller surface areas, are able to adsorb significantly more CO_2 than to the original kerogen, and both original and reacted kerogens have a much higher adsorption capability for CO_2 than CH_4.Therefore, our results support the recently proposed concept of using supercritical CO_2 as a stimulating agent for simultaneous hydrocarbon recovery and carbon sequestration, thus making depleted shale reservoirs as potential sites for CO_2 storage. The observed CO_2-enhanced kerogen transformation may provide an engineering approach to oil/gas extraction from low-mature oil shale such as the Green River Formation. Given the extensive kerogen-CO_2 reaction observed and the volumetric fraction of kerogen in shale, the potential effect of this reaction on the structural integrity of shale as a caprock for a carbon storage system needs to be re-evaluated.

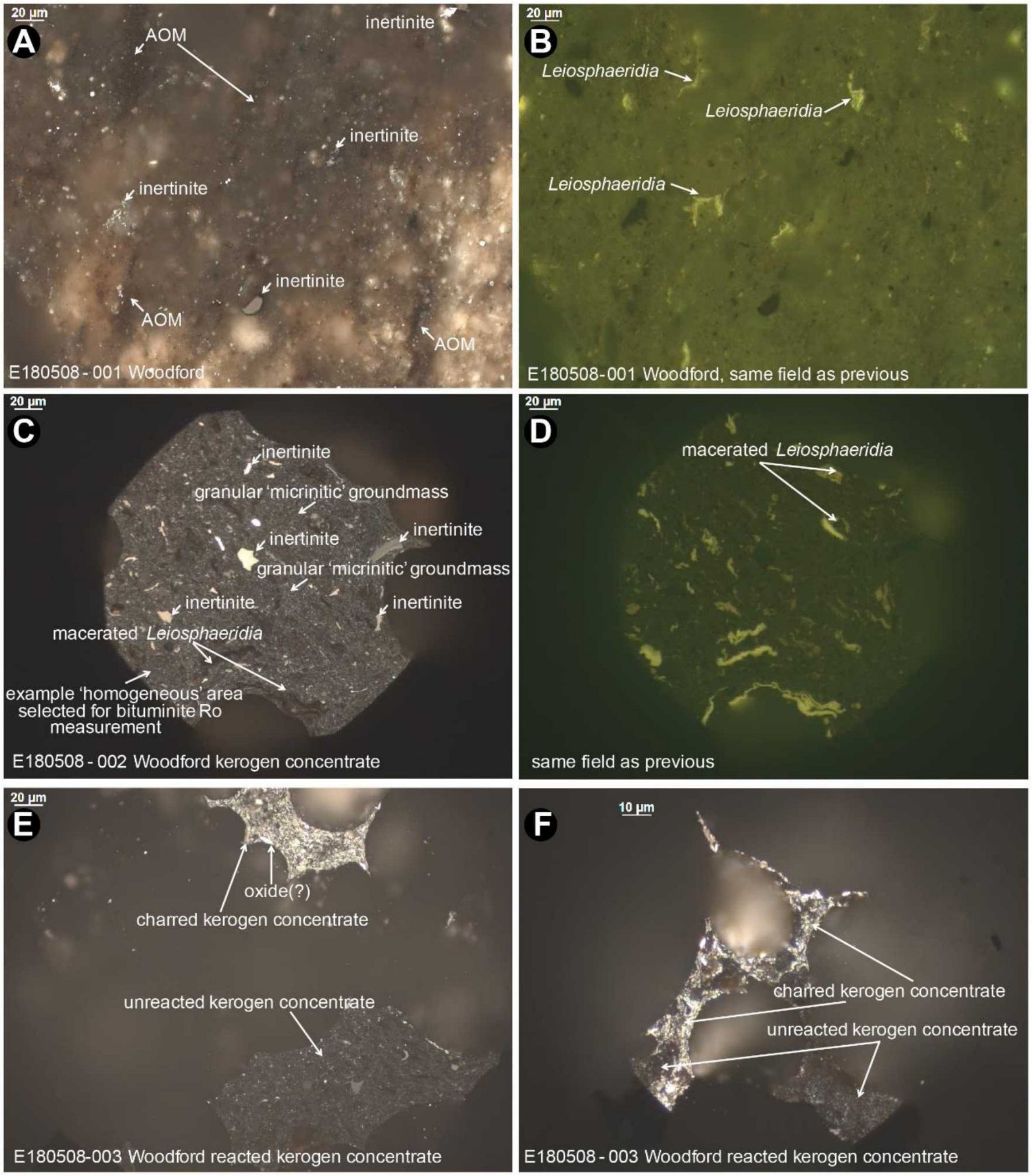

Figure 2. Organic petrography images. A. Original Woodford shale, white incident light under oil immersion. B. Same field as (A) under epi-fluorescence. C. Original kerogen concentrate/extract, white incident light under oil immersion. D. Same field as (C) under epi-fluorescence. E-F. 2nd reacted kerogen concentrate/extract.

3.0 OUTLOOK

- We have initiated the activity on using machine learning for petrographic image analysis. We presented the preliminary result at the American Geophysical Union meeting in December 2018. We plan to report this work in the next quarterly report.
- More MD simulations will be performed on different hydrocarbon fluids and their phase separation in nanopores.

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