Quantifying Interfacial Interactions Between Minerals and Reservoir/Fracturing Fluids

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Authors : Isa Silveira de Araujo and Zoya Heidari, The University of Texas at Austin

Speaker : Isa Silveira de Araujo

Abstract:

Chemical interactions between the injected fluids and the minerals during the fracturing process can affect fluid flow and production. However, there is still a need for understanding the impact of geochemistry on the interactions at the rock-fluids interface, and how these interactions affect wettability of the rock and the fluid flow in organic-rich mudrocks. In this paper, we quantify the mineral-fluid affinity by performing adsorption calculations. Molecular Dynamics Simulations (MDS) are carried out to (i) quantify adsorption of fracturing fluids on the surface of minerals, (ii) perform sensitivity analysis on the composition of fracturing fluid and reservoir temperature on adsorption, and (iii) analyze the spatial distribution of water and chemicals on mineral surfaces. The minerals evaluated include illite, and the fracturing fluid components are methanol, citric acid, sodium chloride and water. Initially, we evaluate the effect of each chemical separately. We generate systems composed of mineral surface in contact with water, salt and each one of the chemicals. Finally, we analyze the complete system containing water, salt, and all additives. MDS are carried out in the canonical (NVT) ensemble at the temperature of 330K to evaluate the adsorption of the fracturing fluid. To quantify the impacts of reservoir temperature, we carry out MDS at temperature of 360K. Results suggest that methanol does not have a strong effect on water adsorption and on the ion spatial distribution on illite surface. We found that citric acid tends to form aggregates and that some cations present in the solution, specially sodium, participate in these citric acid aggregates. When methanol or citric acid are added to the brine solution we observed that mobility of both sodium and water decreased. The effects on mobility of sodium cations were more intense when citric acid was present in the solution. The effects of each additive on the affinity between illite and the fracturing fluids were also investigated. We found that the number of hydrogen bonds between illite and the fluid did not change when additives were added, however we observe a decrease in the number of hydrogen bonds between water molecules when methanol or citric acid were in the solution. The quantification of adsorption in the molecular scale provides fundamental understanding of the electrochemical interactions between the rock surface and the fracturing/reservoir fluids at reservoir conditions, which enables enhanced design of fracturing fluid composition for different reservoir types. This information can also be used to quantify the impacts of injected and reservoir fluids on wettability of the rocks.

Bio:

Isa Silveira de Araujo is a PhD student in the Hildebrand Department of Petroleum and Geosystems Engineering at The University of Texas at Austin. She received her B.S degree in Chemical Engineering from Universidade Federal dos Vales do Jequitinhonha e Mucuri, Brazil, and received her M.S degree in Chemical Engineering from University of Campinas, Brazil in 2019. In her Master thesis she extended the Statistical Associating Fluid Theory (SAFT- VR Mie) equation of state for the calculation of multicomponent adsorption isotherms. In summer 2014, she did a research internship at Texas A&M University and in 2017 she worked as a process engineering intern at Cenibra. Her research interests include petrophysics of unconventional reservoirs and molecular simulations.