Center for Mechanistic Control of Water-Hydrocarbon-Rock Interactions in Unconventional and Tight Oil Formations (CMC-UF) EFRC Director: Anthony R. Kovscek Lead Institution: Stanford University Class: 2018 – 2022

Mission Statement: To seek fundamental mechanistic understanding to achieve control over the various non-equilibrium chemical and physical processes occurring in shale that increases hydrocarbon production while decreasing the amount of produced water, contaminants, and the number of wells drilled.

This EFRC features a tightly integrated fundamental research program combining experimental, theoretical, and numerical science. The plan is comprehensive and interdisciplinary. Importantly, our five overarching research themes foster a fundamental knowledge base from which we learn how to characterize and control single and multiphase reactive transport in shale that is far from equilibrium. We have crafted our plan to unravel heterogeneity and fluid interactions with shale mineral/organic-matter interfaces within the context of a natural extremely disordered system as a function of stress and transport. We exploit and create new imaging and image reconstruction capabilities to explore the largely inaccessible interior of the shale matrix. This is in itself a 'frontier' research focus area. Characterization of nanoporous disordered media before, during, and after reaction is coupled with modeling at length and time scales of interest using advanced models, algorithms, upscaling methods, and computing. The figure below overviews the interplay of length scales, characterization spans. Scale translation is a unifying activity within the research plan as indicated by the progression of scales. Machine learning and data analytics feature throughout the center as important tools for improving physical insight.



Figure. Overlapping length scales of shale features of interest to this EFRC.

From the upper right: water/clay interactions in a 10 nm wide slit pore where water is shaded blue; nanoCT image of shale structure illustrating minerals, and kerogen, outgassed pores; microfractures filled with barite scale; matrix-to-fracture mass transfer; zones of enhanced ductility in heterogeneous shale.

To control materials and processes we must understand mechanisms and use this fundamental knowledge to predict how processes function and evolve with time in diverse chemical and stress state environments. The fundamental science understanding of the coupled chemical and physical processes involving water, hydrocarbons, and substitute fracturing fluids at interfaces in nanoporous media is immature. This Center uses a bottom-up, multiscale, multiphysics, and multidisciplinary approach to investigate disordered nanoporous media incorporating and integrating experiments, structural and chemical characterization before and after reactions, and theory. Scale translation of experimental and model results serves as the centerpiece of our integrative activities.

The center is organized around five cross-disciplinary science goals.

- 1. Develop and exploit advanced multiscale imaging capabilities using x-ray, electron microscopy, and nuclear magnetic resonance techniques to characterize and analyze the fabric of shale at nm to cm scales
- 2. Elucidate the coupled phase behavior, geomechanical, and transport mechanisms of single and multiphase flow through shale using length-scale appropriate experiments and models to understand the controls on flow and transport of water and hydrocarbons.
- 3. Measure, characterize, and model aqueous fluid interactions at shale mineral interfaces and the influence of water composition on matrix, microfracture, and fracture fluid transfer and transport.
- 4. Characterize the mechanisms of viscoplasticity and ductility of shale when exposed to alternate hydraulic fracturing fluids such as CO₂, N₂, and aqueous foams of CO₂ and N₂.
- 5. Enable translation of physical and chemical mechanisms to assess their influence at macroscopic length and time scales using advanced algorithms and modeling that take advantage of emerging high-performance computing with heterogeneous processors and complex memory hierarchies.

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