Center for Mechanistic Control of Water-Hydrocarbon-Rock Interactions in Unconventional and Tight Oil Formations (CMC-UF)
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***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.*

CMC-UF features a tightly integrated fundamental research effort combining experimental, theoretical, and numerical science. We are motivated by the economic, strategic, and environmental importance of unconventional formations, i.e., shale resources, and the lack of mechanistic understanding of coupled transport, reaction, and mechanical processes in such natural nanoporous media interlaced with fractures, Fig. 1. Fundamental physical and chemical understanding is foundational to achieve first-order improvements in environmental outcomes and recovery.

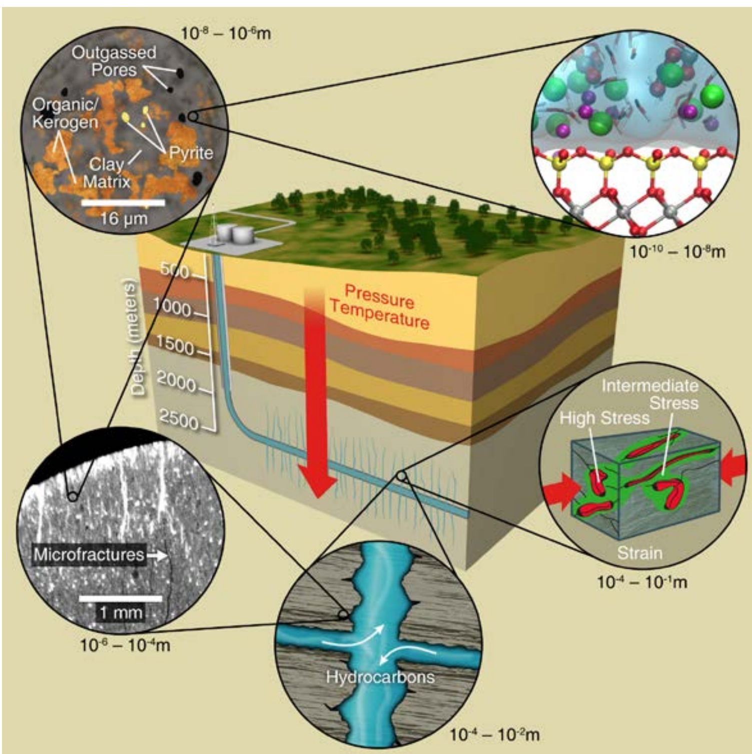

Fig. 1. Overlapping length scales of shale features of interest to CMC-UF. *From the upper right*: water/clay interactions in a 10 nm wide slit pore where water is shaded blue; nanoCT image of shale structure illustrating minerals, kerogen, and outgassed pores; micro-fractures filled with barite scale; matrix-to-fracture mass transfer; zones of enhanced ductility in heterogeneous shale.

Our research approach is comprehensive and interdisciplinary. Importantly, five overarching research themes (i.e., discipline-specific expertise) are crosscut by seven multidisciplinary, synergistic research activities to foster acquisition of fundamental knowledge, as shown in Table 1. CMC-UF has made significant progress in unraveling the interplay of material heterogeneity, transport through heterogeneous structures, and fluid interactions with shale mineral/organic-matter interfaces within the context of a natural disordered system as a function of stress and transport process.

We are exploiting and creating new imaging and image reconstruction capabilities before, during, and after reaction to explore the largely inaccessible interior of the shale matrix. We employ X-ray computed tomography (CT), positron emission tomography (PET), scanning electron microscopy, scanning transmission electron microscopy and nuclear magnetic resonance (NMR) to achieve resolution from cm to nm length scales of reactive transport processes. We are pioneering chemical and physical description of reactive imbibition where rates of mass transport are of the same order as rates of chemical reaction. Importantly, we are developing and applying machine learning and data analytics to achieve image super resolution and to facilitate interpretation among measurement modalities.

Machine learning also features in our efforts to translate the impact of physical phenomena across scale. Convective and diffusive mass transfer is studied jointly with imaged dynamic experiments employing microfluidics, x-ray CT, and PET. Experiments are conducted in concert with at-scale numerical models including molecular dynamics, direct numerical simulation, lattice Boltzmann methods, and continuum formulations. Translation of the importance of physical mechanisms across length and time scales is a unifying activity within the research plan as indicated by the progression of scales in Fig. 1 and the activities in Table 1.

Table 1. Matrix of research expertise cross cutting the 7 major synergistic research activities in CMC-UF. All activities incorporate experimental measurements, theory development, and activities to translate results across length and time scales.

<table>
<tr><th></th><th colspan="5">Research expertise</th></tr>
<tr><th></th><th>Characterization methods</th><th>Transport processes</th><th>Reactivity at interfaces</th><th>Geomechanics</th><th>Translation</th></tr>
<tr><th rowspan="7">Synergistic activities</th><td colspan="5">Mechanics of shale in the presence of reactive and nonreactive aqueous and nonaqueous fluids</td></tr>
<tr><td colspan="5">Reactive imbibition of aqueous fluids in concert with evolution of tight matrix pore and microfracture structure</td></tr>
<tr><td colspan="5">Reactive transport in fractured media from the pore to the continuum scale</td></tr>
<tr><td colspan="5">Sorption and capillary condensation in nanoporous geomaterials</td></tr>
<tr><td colspan="5">Phase transitions in tight materials in comparison to bulk properties</td></tr>
<tr><td colspan="5">Probing advection and diffusion in nanoporous matrix from pore to pore network to core scale</td></tr>
<tr><td colspan="5">Matrix-fracture interactions of tight matrix communicating with microfractures in the context of transport, reactions, and mechanics</td></tr>
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