Center for Mechanistic Control of Unconventional Formations (CMC-UF)
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Mission Statement*: to garner cross-cutting geoscience knowledge to achieve mechanistic control over the strongly coupled nonequilibrium physical and geochemical processes in extreme geological environments including shale, mudstone, marls, and other tight rocks with nanoscale pores. Collectively, these are referred to as unconventional formations and all subsurface storage formations are sealed by an unconventional formation.*

Unconventional formations will play an outsized role in the transition of energy from large greenhouse gas emissions to renewables and net-zero emission technologies in the coming decades. Importantly, unconventional formations serve as the geological seals atop conventional subsurface formations, Fig. 1-1, in addition to being a significant source of low-carbon intensity natural gas. This functionality implies confinement of sequestered CO_2 and storage of intermittent renewable energy (e.g., green hydrogen or compressed air) beneath seals as well as isolation of nuclear waste. While unconventional formations are ubiquitous throughout the subsurface, our fundamental and engineering science knowledge of them is limited by their nanoporous structure, extreme heterogeneity that spans at least 10 orders of magnitude spatially, and significant reactivity. Four challenges inhibit a system-level understanding of unconventional formations: (1) the physics of fluid transport and phase behavior are poorly understood due to dominant molecular interactions between rock/fluid molecules under confinement; (2) their mechanics, especially in the presence of nonaqueous fluids such as H_2 and CO_2, requires significant exploration; (3) reactivity of solid/fluid interfaces is governed by complex processes that are strongly coupled to transport and mechanics; and (4) the lack of scale separation prevents a reliable (closed) description of physicochemical processes at any single scale of observation. Our fundamental science goals G1—G5, and research plan below, address these challenges directly.

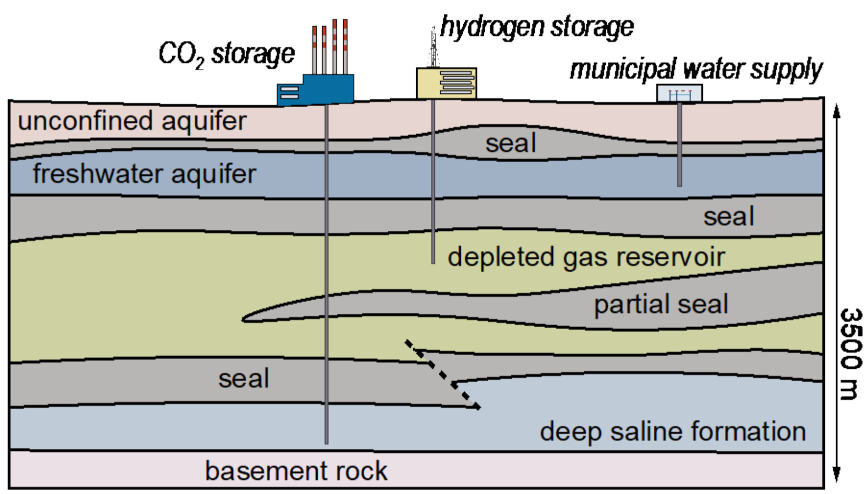

Fig. 1-1. Typical geological strata with seals (unconventional formations). Gas reservoir is repurposed for seasonal H_2 storage. The reservoir seal prevents vertical H_2 movement. Anthropogenic CO_2 is injected into a deep saline formation for secure storage. Top and bottom seals confine CO_2 to the formation.

Seal integrity and storage capacity are subject to geochemical interactions at shale-mineral interfaces, and confined phase and transport behavior that emerge out of intricate interactions in the mechanically stressed nanoporous structure. This structure is heterogeneous across scales, from nm to m. The fundamental understanding that is needed to assemble this complex puzzle requires exploration of the impact of microscale heterogeneity and exploiting transformative advances in experimental and computational modeling capabilities across scales. These are important to unraveling the role of larger-scale structural heterogeneity and variability that could be important for real-world full-scale projects including faults and weaker sections of a cap rock. CMC-UF's **approach is multiscale and multiphysics** while incorporating and integrating experiments, characterization before and after reactions, theory, and computational modeling efforts. Our research expertise is interdisciplinary, collaborative, and aligned with our science goals (**G1—G5**): (1) multiscale characterization and imaging; (2) multiphase, multiphysics transport processes; (3) reactivity at fluid/solid interfaces; (4) geomechanics; and (5) scale translation.

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