Shales at all scales: Exploring coupled processes in mudrocks

Geological Carbon Storage
Relies on structural and capillary trapping of CO₂ in the subsurface. Caprock performance is the key to successful storage. Shale is one of the most common rock types that comprise caprock.

The CFSES Research Challenges
1. Sustaining large storage rates.
2. Using pore space efficiently.
3. Controlling undesired/unexpected behavior.

Rationale for this review paper
The development of conceptual models for the coupled thermal-hydraulic-mechanical-chemical-biological (THMCB) processes in shale formations presents a major scientific challenge. We assessed outstanding and fundamental issues in shale science and developed recommendations for future research and integrating multi-disciplinary data for models appropriate for multi-scale, multi-physics coupled processes in shale.

Publication:
Unique physical and chemical characteristics of shale

Physical
- Fine-grained minerals.
- Nanoporosity.
- Dual-porosity pore networks.
- Layering from nm to tens of cm.
- Low permeability fabric.
- Heterogeneity from nm to km.
- the only “common” rock type, where all four (Darcian, Fickian, Fourier and Ohmic) diffusion processes can co-exist.

Chemical
- Wide range of mineralogical compositions.
- High salinity brines.
- Organic matter.
- Nano-confinement effect on chemical reactions.
- Low activity of water.
Why is THCMB process coupling important for shale?

In coupled processes observed in shale formations one of the key variables is volume change. Microscopic processes of swelling and shrinking of clay minerals results in macroscopically observed expansion and contraction of shale beds. Volume changes control the state of stress, which leads to yield (shearing and fracturing) and changes in geometry of pore and fracture networks, and resulting changes in permeability and diffusivity. Understanding the THCMB process coupling and feedbacks necessitates quantifying the volume changes, governing processes and their rates and incorporating them into numerical models.

**Issues of temporal and spatial scales:** Methods to honor the multi-scale heterogeneity in models that predict the response of shales to natural and induced physical and chemical changes is one of the key challenges of shale science.
Methodologies for understanding process coupling

Successful modeling approaches

- Dynamic consolidation problems with elastoplastic deformation and finite element modeling (FEM).
- Quasi-static discrete element models (DEM) coupled with conjugate lattice network flow.
- Basin petroleum system modeling, incorporating Knudsen diffusion and gas slippage (in addition to Darcy flow) into reservoir models for shale.
- Lattice Boltzmann (LB) approaches for coupled multi-component reactive flow and transport with the feedback between pore structure changes and flow processes.
Coupled processes in shale: future research needs

### Data and Classification Schemes
- Data from shale formations at *in situ* pressure and temperature conditions.
- Methodologies for merging multidisciplinary datasets at different length and time scales.
- Developing classification schemes for mudrocks, and further understanding of the material transport and cementation mechanisms during shale deposition and diagenesis.
- Establishing the range of sizes for REVs, different for kerogen, clay mineral-rich components, and individual lithofacies, that are controlled by the unique depositional and diagenetic history.

### Anisotropy
- Developing methods for integrating rock anisotropy into geomechanical analysis, modeling of mechanical interfaces, and developing new constitutive laws describing stress-strain relationships.
- Separating competing sources of anisotropy in rock and fluid flow, and how seismic signals change as a function of stress and fluid conditions. Test whether seismic data can differentiate chemical, fluid and stress alteration of fractures.

### Nano-confinement effects
- Developing new thermodynamic databases, and theory for predicting shifts in chemical kinetics under nano-confinement.

### Predictive Modeling
- Incorporating coupled behavior in locally heterogeneous shale: 2-way coupling of solid solvers with multiphase reactive flow/transport codes, incorporating reaction feedback to the permeability and mechanical properties.
- Development of porosity-permeability relationships.
- Methods for computing the effect of flow on the mechanical constitutive behavior of shale (as partially-drained or undrained medium).
- Flow models to incorporate multi-porosity system behavior.
- Additional laboratory data on coupled processes for calibration and verification of these coupled models.

### Scientific Achievement
Identified key coupled processes in shale, and developed multi-disciplinary future research needs.

### Significance and Impact
Insight on the unique physical and chemical properties of shale, and the evolution of these properties in response to perturbations, including injection of CO₂.