



Invited review

Shales at all scales: Exploring coupled processes in mudrocks



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ABSTRACT

Fine-grained sedimentary rocks – namely mudrocks, including their laminated fissile variety – shales – make up about two thirds of all sedimentary rocks in the Earth's crust and a quarter of the continental land mass. Organic-rich shales and mudstones are the source rocks and reservoirs for conventional and unconventional hydrocarbon resources. Mudrocks are relied upon as natural barriers for geological carbon storage and nuclear waste disposal. Consideration of mudrock multi-scale physics and multi-scale spatial and temporal behavior is vital to address emergent phenomena in shale formations perturbed by engineering activities. Unique physical characteristics of shales arise as a result of their layered and highly heterogeneous and anisotropic nature, low permeability fabric, compositional complexity, and nano-scale confined chemical environments. Barriers of lexicon among geoscientists and engineers impede the development and use of conceptual models for the coupled thermal-hydraulic-mechanical-chemical-biological (THMCB) processes in mudrock formations. This manuscript reviews the THMCB process couplings, resulting emergent behavior, and key modeling approaches. We identify future research priorities, in particular fundamental knowledge gaps in understanding the phase behavior under nano-scale confinement, coupled chemo-mechanical effects on fractures, the interplay between physical and chemical processes and their rates, and issues of non-linearity and heterogeneity. We develop recommendations for future research and integrating multi-disciplinary conceptual models for the coupled multi-scale multi-physics behavior of mudrocks. Consistent conceptual models across disciplines are essential for predicting emergent processes in the subsurface, such as self-focusing of flow, time-dependent deformation (creep), fracture network development, and wellbore stability.

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Contents

1.	Introduction: shale architecture, heterogeneity, and coupled processes	133
1.1.	Significance of mudrocks, and laminated mudrocks – shales	133
1.2.	Key physical and chemical characteristics of shales.	133
1.3.	Why is THMCB process coupling important for shale?	134
2.	Methods	136
3.	Methodologies applied to coupled processes in shale	136
3.1.	Post-depositional physical and chemical processes in shale (diagenesis)	136
3.2.	Physical and chemical controls on fracturing in shale.	137

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3.3. Fluid flow in multi-porosity systems	141
3.4. Nano-scale confinement, activity of water, and pore-scale coupled processes in shale	144
3.5. Equilibrium-disequilibrium transitions in perturbed shale	147
4. Conclusions: approaches for coupled process studies and future research needs.	147
4.1. Summary of applied approaches/methodologies.	147
4.2. Coupled processes in shale: future research needs.	148
Acknowledgements	149
References	149

1. Introduction: shale architecture, heterogeneity, and coupled processes

1.1. Significance of mudrocks, and laminated mudrocks – shales

Sedimentary rock containing more than 50% (by weight or volume) of particles less than 62.5 μm in size is known variously as shale, siltstone, claystone, mudstone, and is cumulatively referred to as mudrocks (Folk, 1980; Milliken, 2014; Tucker, 2009). Some workers apply “shale” narrowly to refer to the visibly laminated, fissile variety of this sedimentary rock, but in this paper we apply this term as the overall name for the broad class of fine-grained layered sedimentary rocks, and, where appropriate, use it interchangeably with the term “mudrock” (Boggs, 2006). Shale constitutes around two-thirds of the sedimentary record of planet Earth (Garrels and Mackenzie, 1969; Blatt, 1982), and a quarter of the continental land mass (Jin et al., 2014). In some portions of sedimentary basins, distant from the principal axes of sediment transport, the abundance of mudrocks may approach 90% of the local sediment volume (Galloway et al., 1982). Shales are volumetrically dominant in both marine and terrigenous successions, and host significant portions of the fluid-rock interactions controlling fate and transport of elements in the upper crust (Milliken, 2004), and atmosphere – e.g., chemical weathering of shale has been shown to serve as a long-term global sink for carbon dioxide (CO_2) (Jin et al., 2014). Thus, shale properties are key controls on interactions of the atmosphere, hydrosphere and sedimentary lithosphere in many contexts, and are crucial reservoirs for unconventional oil and gas production, top seals for conventional hydrocarbon traps and geological CO_2 storage (GCS), and isolation of nuclear and other high-level wastes.

In each case, shales are of interest both as barriers to fluid flow (seals) and as rock units that support flow of their contained fluids (reservoirs). Accelerated growth of information on Earth's most abundant sedimentary rock highlights key gaps in our understanding of this rock type. The development of conceptual models for the coupled thermal-hydraulic-mechanical-chemical-biological (THMCB) processes in shale formations presents a major scientific challenge. In this paper we assess outstanding and fundamental issues in shale science that present obstacles to practical management of shales as seals, reservoirs, and source rocks. We develop recommendations for future research and integrating multi-disciplinary data for models appropriate for multi-scale, multi-physics coupled processes in shale.

1.2. Key physical and chemical characteristics of shales

The physical and chemical properties of shales are controlled by their depositional environment, post-depositional diagenetic history, and engineering activities. In general terms, shales are commonly distinguished by their layered low-permeability fabric and composed of fine-grained minerals. One of the primary components of source rock shale is organic matter (e.g., kerogen). Porosity and pore sizes of shale are variable; however, nano-pores comprise a large fraction of the total porosity (Ross and Bustin, 2009; Loucks et al., 2009; Chalmers et al., 2012; Nelson, 2009).

Historically, shales have been strongly identified by their clay mineral content because clay minerals are a component that controls the

physical behavior of shale at scales ranging from field and laboratory to the nano-scale (Potter et al., 2005). Although most shales contain at least a few volume percent of clay minerals, petrographic inspection by high-resolution methods shows that non-phyllonite minerals such as quartz, feldspar, and calcite dominate in many shale lithologies and that organic components contribute additional complexity (Cook and Sherwood, 1991; Dean et al., 1985; Aplin and Macquaker, 2011). Compositional classification of shales has not, to date, benefited from a level of community consensus that is analogous to the widely applied classifications of sandstones and limestones (Milliken, 2014; Lazar et al., 2015; Bourg, 2015). It is clear however, that shales display a range of mineralogical compositions that encompass that of sandstones and limestones in addition to actual clay-mineral-rich rocks (Milliken, 2014).

Recent advances in understanding shale heterogeneity at many scales have been founded, in part, on a heightened appreciation of the nature of fundamental components (grains, cements, and grain replacements) as revealed by high resolution electron microbeam imaging (Wawak et al., 2013). Both observational (Lazar et al., 2015) and experimental (Schieber et al., 2007) approaches demonstrate that the physical sedimentology of fine-grained sediments entails a complex set of advective transport mechanisms as well as gravity settling, leading to distinctive textural and fabric characteristics at the bed scale that can be used to infer depositional conditions (Lazar et al., 2015). In this paper we use the term “texture” (rock microstructure) to refer to the combination of properties, including maturity, pore characteristics, fragment shape, roughness, composition, sorting, and diagenetic features – matrix and cement (Vernon, 2004).

Pores in shale manifest at a variety of sizes within kerogen (organic material), the inorganic mineral matrix, and fractures formed during natural processes or engineering activities (Akkutlu and Fathi, 2012; Saraji and Piri, 2015). The structures of pores reflect depositional processes and also the chemical and mechanical diagenetic processes associated with burial. In organic-rich shales, thermal maturation results in kerogen cracking and production of liquid hydrocarbons and gas, which also modifies the nature of porosity within organic components associated with these rocks.

Pore waters comprise approximately 20% by volume of most sedimentary basins (Mondol et al., 2007; Kharaka and Hanor, 2014). The salinity of pore waters in petroleum reservoir rocks, including values reported for shale and tight reservoirs with *in situ* temperatures of ~ 20 – 150 $^{\circ}\text{C}$ and fluid pressures of ~ 100 – 1000 bar, varies widely from approximately 1000 mg L^{-1} to over $400,000$ mg L^{-1} total dissolved solids (TDS) (Kharaka and Hanor, 2014). Detailed inorganic and organic chemical analyses, together with measurements of stable and radioactive water and solute isotopes have shown that the formation waters in sedimentary basins are dominantly of local meteoric or marine connate origin. However, bittern – residual evaporated seawater, geologically old meteoric water, and especially waters of mixed origin are important components in most sedimentary basins (Kharaka and Hanor, 2014). During diagenesis, the original waters of deposition evolve to Na–Cl, Na–Cl– CH_3COO^- , or Na–Ca–Cl-type waters by a combination of several processes including (1) dissolution of evaporites, especially halite; (2) diffusion and advection, especially in and near salt domes; (3) reflux and incorporation of bitterns; (4) dissolution,

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