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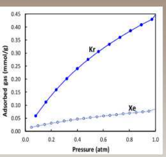

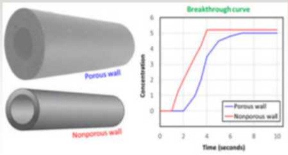

Predicting Gas Transport in the Subsurface

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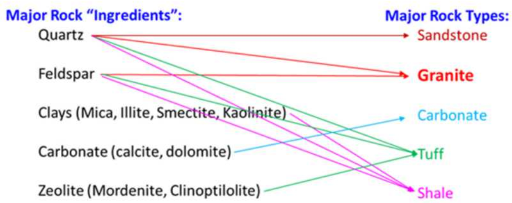
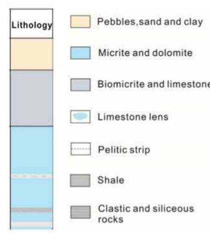
Objective/Problem to Be Addressed

- Apply multiscale modeling and laboratory experiments to better understand the impacts of host rock properties on gas transport in the subsurface. Create a bridge to engineering codes used to predict flow and transport in porous media
- **Problem.** Subsurface gas transport behavior can show significant deviations from conceptual models that do not include the chemical or physical properties of the host rock.
  - Existing gas transport codes: input parameters derived from core samples, assume homogeneous rock phases.
  - Transferability of field data from test sites with similar geologic properties such as permeability.
- **Solution:** Focus on gas properties in pure mineral phases.

Gas properties in pure mineral phases and **"synthetic rocks"** → Predicted transport in different lithologies (shale, granite, tuff)



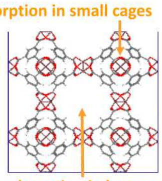


Minerals **2018**, *8*, 516

Research Strategy

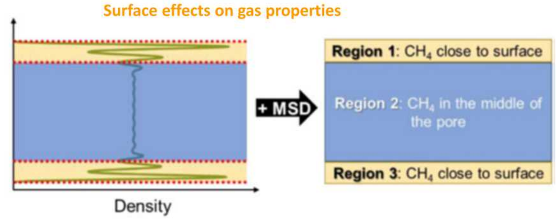
- **Goal:** Obtain a fundamental understanding of gas migration in mineral phases, particularly for which **adsorption** could affect the transport properties depending on gas-rock interactions.
- **Science Question:** To what extent do surface effects determine the relevance of pores and pore walls on gas transport in micropores?
- **Hypothesis.** Nonadsorbed (diffuse) species will behave as a bulk fluid or gas beyond a critical distance from the surface.
- Three factors that control subsurface gas transport:
  - Pore size and fracture surface effects on gas adsorption and transport.
  - Gas affinity for mineral surfaces along the transport pathway, including competitive adsorption effects.
  - The effect of gas-water-mineral interactions on adsorption and diffusion.

Strong adsorption in small cages



No adsorption in large pores

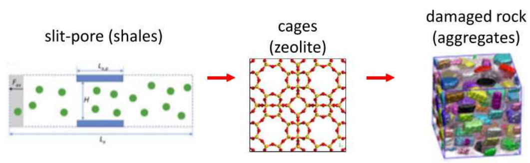
Surface effects on gas properties



J. Chem. Theory Comput. **2018**, *8*, 516

Molecular Dynamics (MD) Modeling

Effect of (gas and pore) size interactions on adsorption and transport



Transport complexity

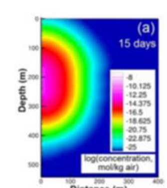
static (equilibrium) → pressure-driven flow (non-equilibrium)

Experimental Measurements

- Characterization. Pore size distribution, porosity, water content.
- Measurements
  - Adsorption/desorption (temperatures and water content)
  - Breakthrough
  - Diffusion

Transport Modeling

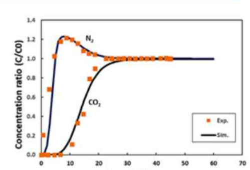
- Pressure-induced flow (advection) and diffusion are primary transport modes
- Partition coefficient (K_d) and diffusion coefficient inputs from Tasks 1 and 3
- Output will be gas concentration (saturation) profiles as a function of time
- Stochastic sampling of hydrogeologic input parameters
  - **Porosity**
  - **Permeability**



Example of a 2-D concentration profile at 15 days for an initially pressurized subsurface gas source. (*Sci. Reports* **2015**, *5*, 18383)

Breakthrough Modeling

Bridge between MD modeling and column experiments



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