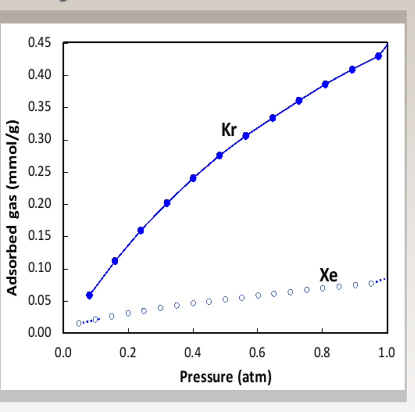

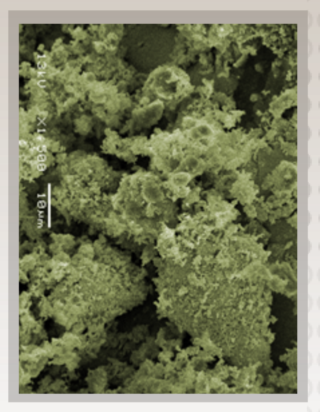

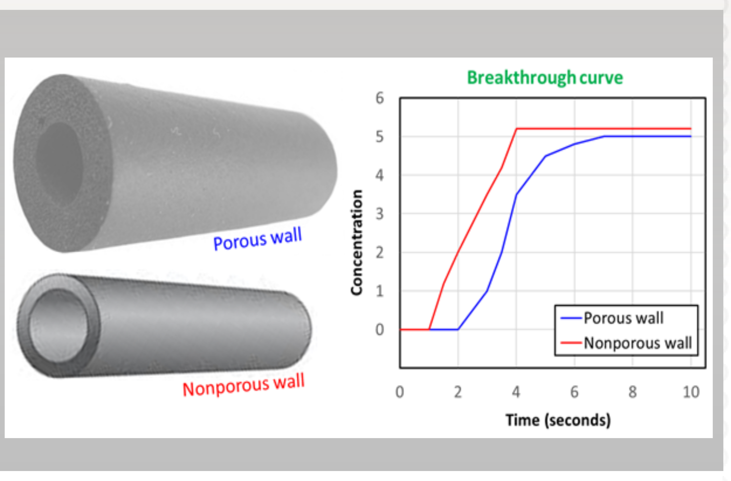

Predicting Gas Transport in the Subsurface

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Todd Zeitler, Geotechnology & Engineering
Hongyou Fan, PM, Geochemistry

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, or assume homogeneous rock phases.
  - Transferability of field data from test sites with similar geologic properties such as permeability.

Research Strategy

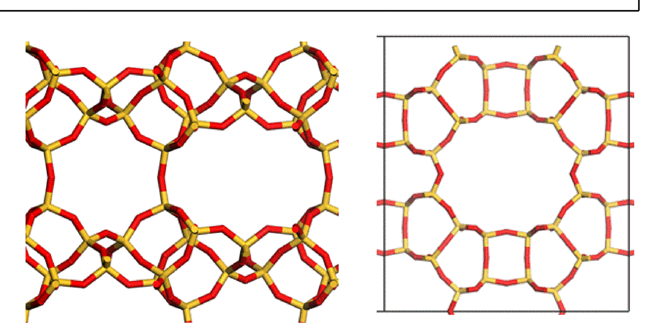
- Obtain a fundamental understanding of gas migration in mineral phases, particularly for which **adsorption** could affect the transport properties.
- Focus on gas properties in pure mineral phases.

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

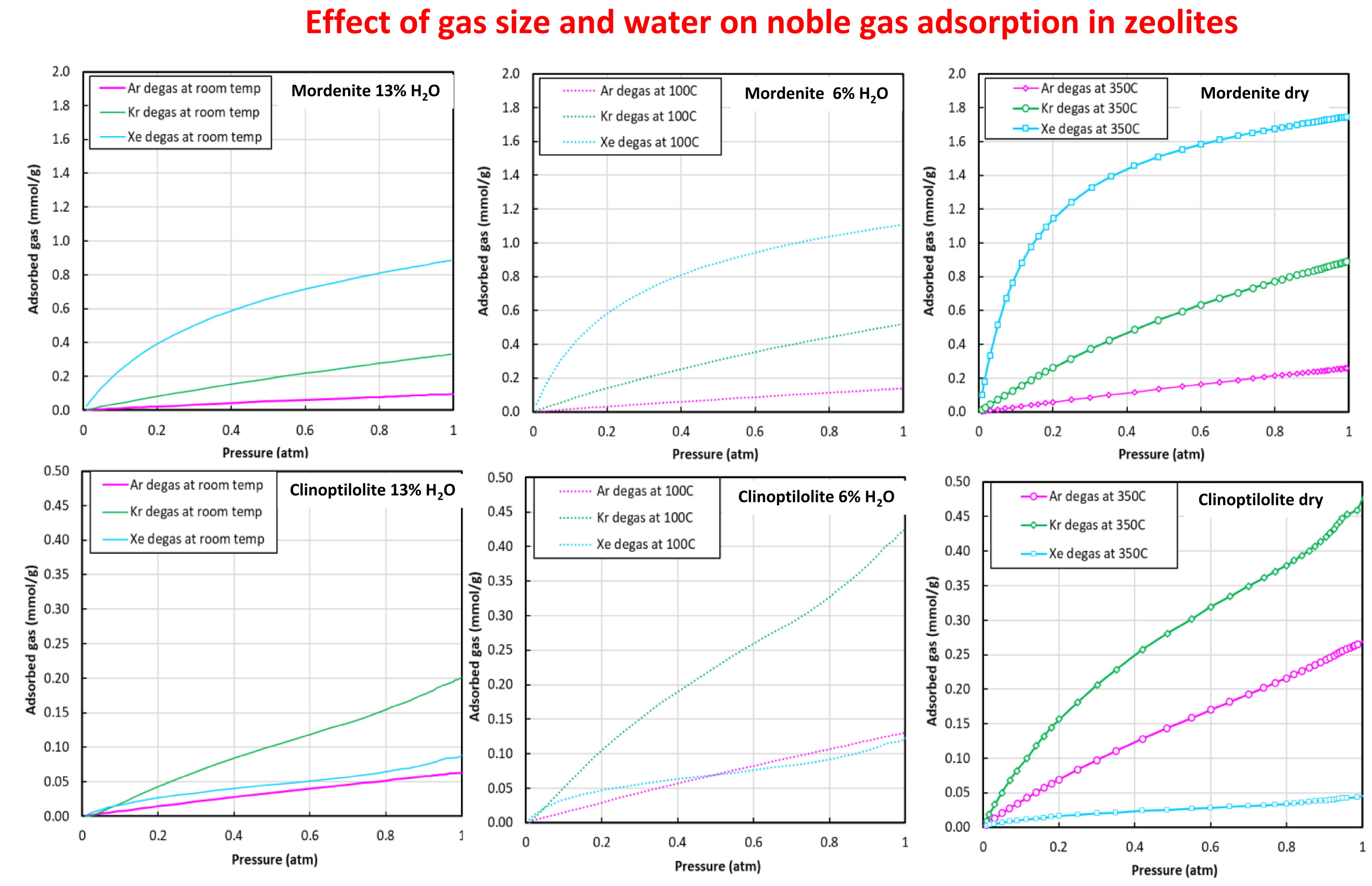
- **Science Question:** To what extent do surface effects determine the relevance of pores and pore walls on gas transport in micropores?
- Three factors that control subsurface gas transport: 1) pore properties such as size and tortuosity, 2) adsorption, and 3) water.

Experimental Measurements of Gas Uptake in Zeolites

Cage	Clinoptilolite	Mordenite
Small	3.3 Å – 4.8 Å	3.6 Å – 4.8 Å
Large	3.3 Å – 5.5 Å	6.3 Å – 6.5 Å

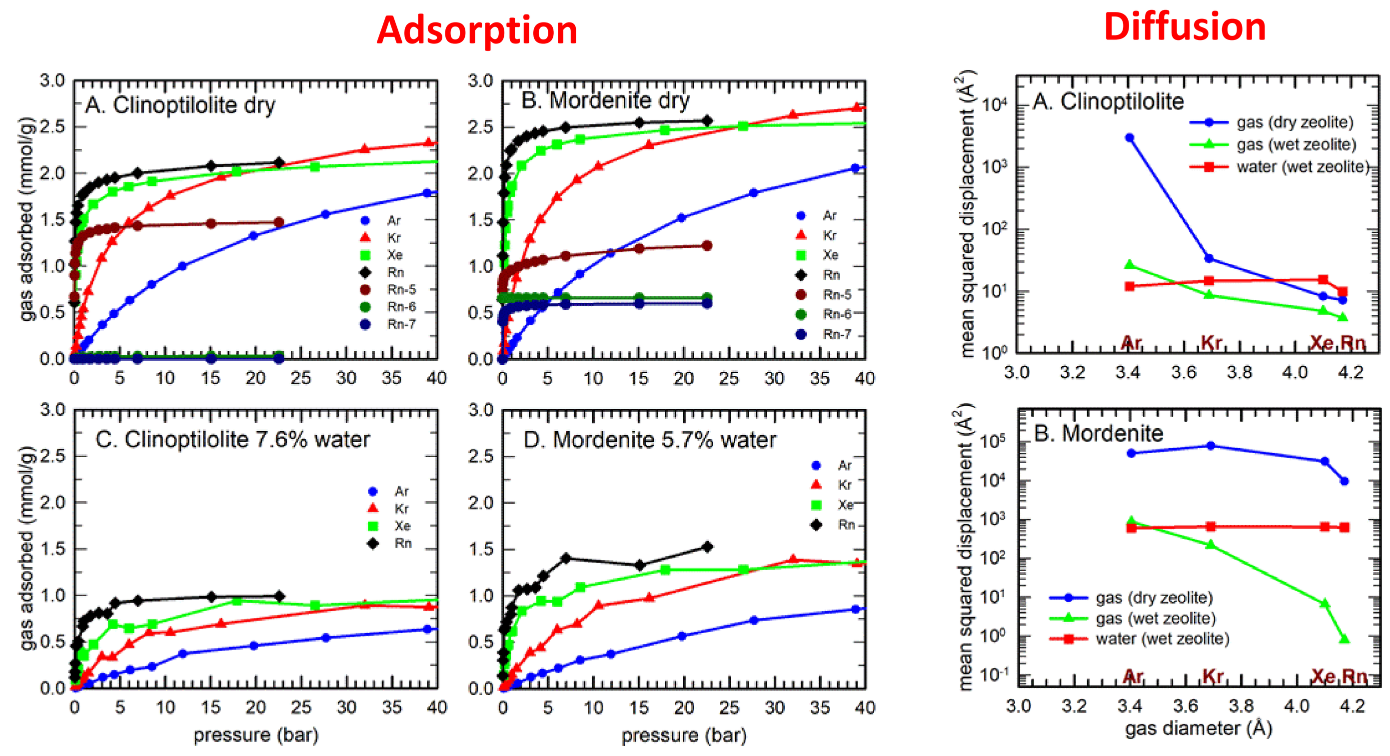


Effect of gas size and water on noble gas adsorption in zeolites



- Mordenite (large cages): expected adsorption trend (Ar < Kr < Xe), adsorption increases as water content decreases.
- **Clinoptilolite (small cages): reverse selectivity (Kr > Xe) in dry or wet environments. Initial uptake of Kr and Xe are similar.**

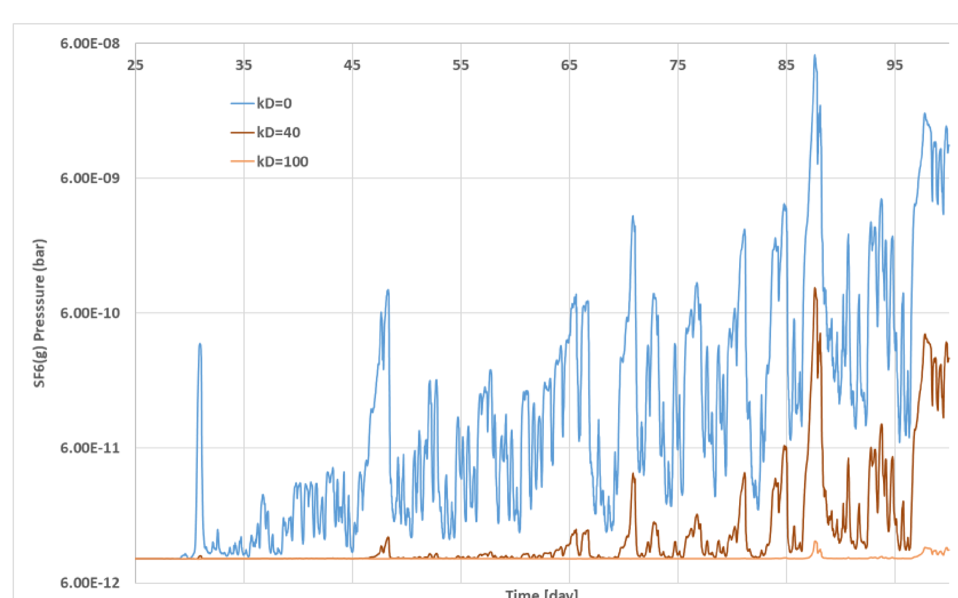
Molecular Dynamics (MD) Modeling of Zeolites



- Large cage in mordenite can accommodate all gases with increased gas mobility.
- Water greatly decreases adsorption and gas mobility.
- No reverse adsorption selectivity (Kr > Xe) seen in clinoptilolite, but Xe has limited mobility in dry and wet environments. **Matches experimental observations.**

Transport Modeling at the Field Scale

- Pressure-induced flow (advection) and diffusion are primary transport modes
- Stochastic sampling of hydrogeologic input parameters
  - **Porosity**
  - **Permeability**
  - **Partition coeff. (K_d)**
  - **Diffusion coeff.**



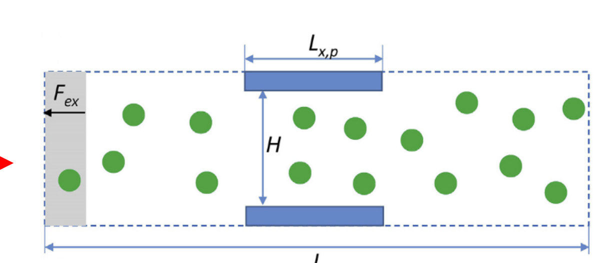
Example of delayed breakthrough due to increasing partition coefficient (K_d in kg_{water}/m^3_{bulk}). This shows the potential impact of gaseous adsorption along a fracture pathway to the surface.

Publications and Presentations

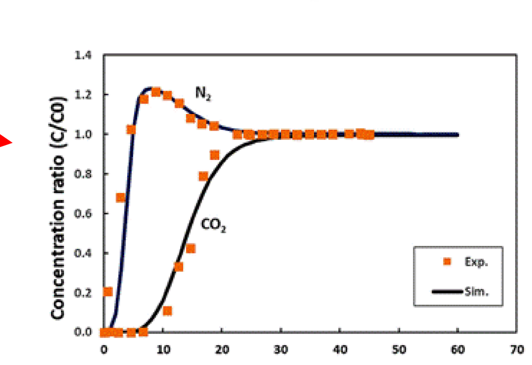
- 2 presentations at 2020 Goldschmidt Conference
  - Xu. Effects of Mineral Adsorption on Subsurface Gas Transport.
  - Zeitler. Parameter Sensitivity in Subsurface Gas Transport Calculations.
- Manuscript in prep. Xu et al. Zeolite Adsorption Effects on Subsurface Gas Transport

Plans for FY21

- Non-equilibrium MD (pressure-driven flow).
- Experiments: gas properties in mineral mixtures.
- Lab-scale breakthrough modeling.
- Transport modeling: parameter sensitivity and gas mixtures.



He et al, 2017



Ben-Mansour et al, 20128

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