Used Fuel Disposition Campaign

Neutron investigation of pore structure and water dynamics in natural and engineered materials for nuclear waste repository systems

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Outline

Problems

- Water movement and transport in low permeability media (e.g., clay, rock salt, cement, cement-clay)
- Topic # P4 & # P5, UFDC Natural system evaluation R&D plan

Approaches

- Small-angle neutron scattering (SANS)
- Inelastic incoherent neutron spectroscopy (IINS) with filter difference spectrometer (FDS)

Updated Results

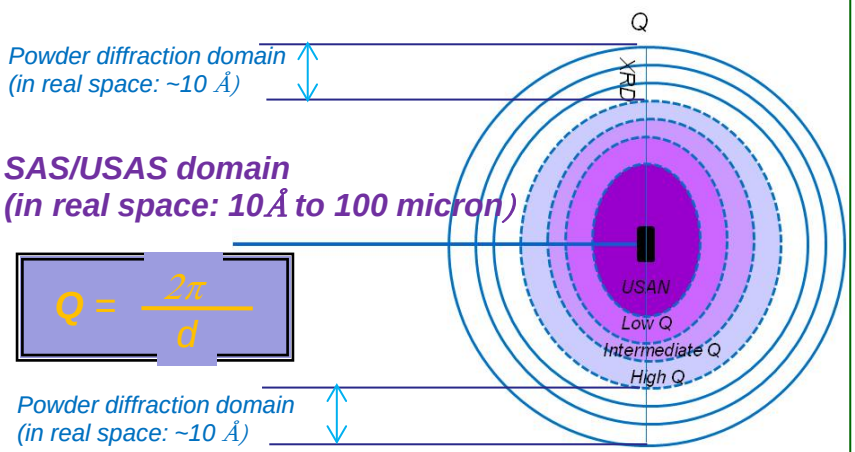
- Pore characterization of cement-clay barrier material
- Water characterization in Permian rock salt at elevated temperature

Path-Forwards

- Capability development
- UFD relevance & Broad applications

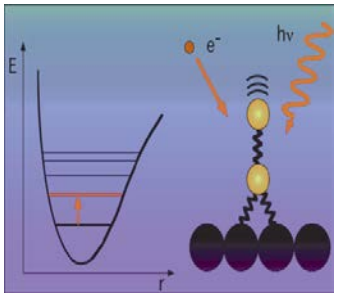
Techniques

Principle

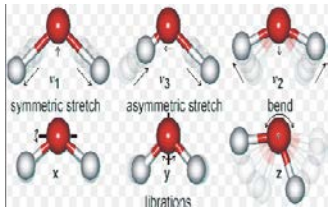


IINS-FDS

$$E_s = E_i - E_f$$



❖ ***Vibrational mode of water***



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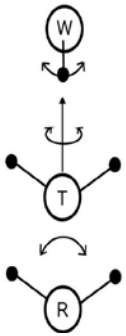
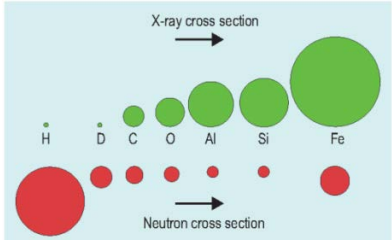
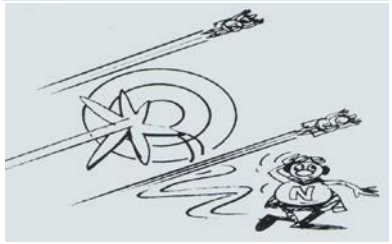
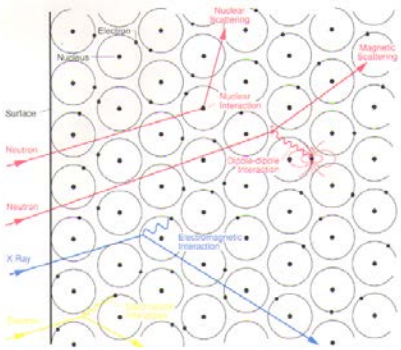


Why neutron

❖ ***Neutrons are very sensitive to hydrogen***







Scattering interactions mechanism (R. Pynn 1990)

- No charge
- Nuclear and magnetic interactions

❖ ***Non-destructive and high penetration (flexible sample environment)***

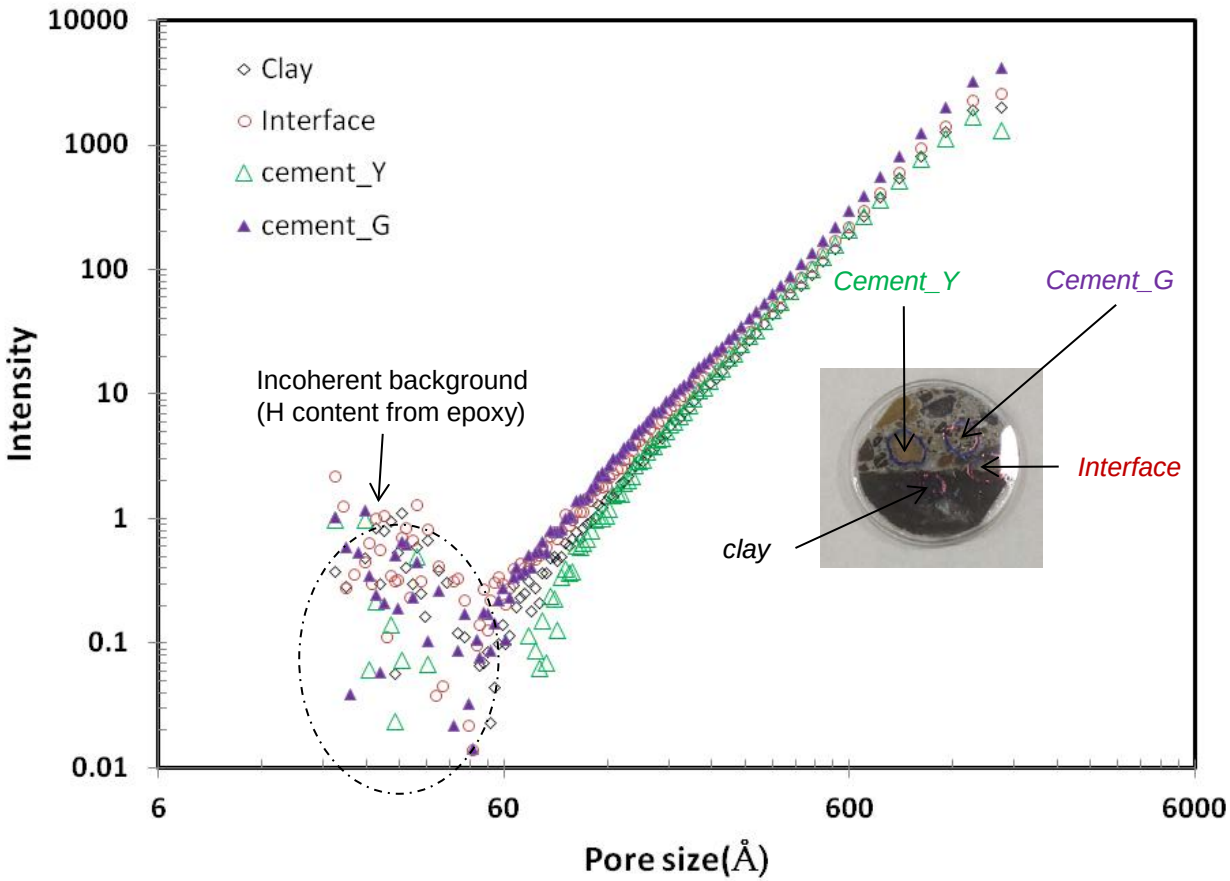
❖ ***Contrast matching possible (Different isotopes scattering differently)***

Pore characterization of cement-clay barrier material

SANS

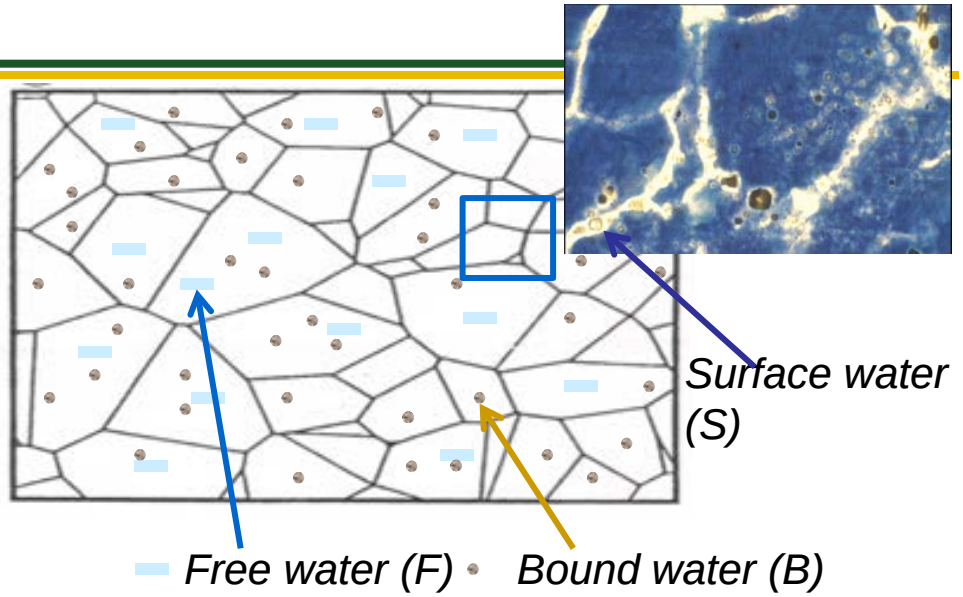
- Influence of Cement on Clay in a deep geological repository
- Reactive transport in Complex System
  - Heterogeneous
  - Dynamic
- To evaluate the effects of Secondary Mineral Precipitation on seal performance

- SANS data analysis indicates that precipitates occurred at the interface
- Interface pore feature close to small granular geometric medium in cement
- SANS can sample specific areas



Forms of water in rock salt

1. ***Free water (F),*** *as fluid inclusion*
2. ***Bound water (B)****, as chemically bound water (crystallized and constitutional water, and physically bound water)*
3. ***Surface water (S)*** *present as grain-boundary fluids*



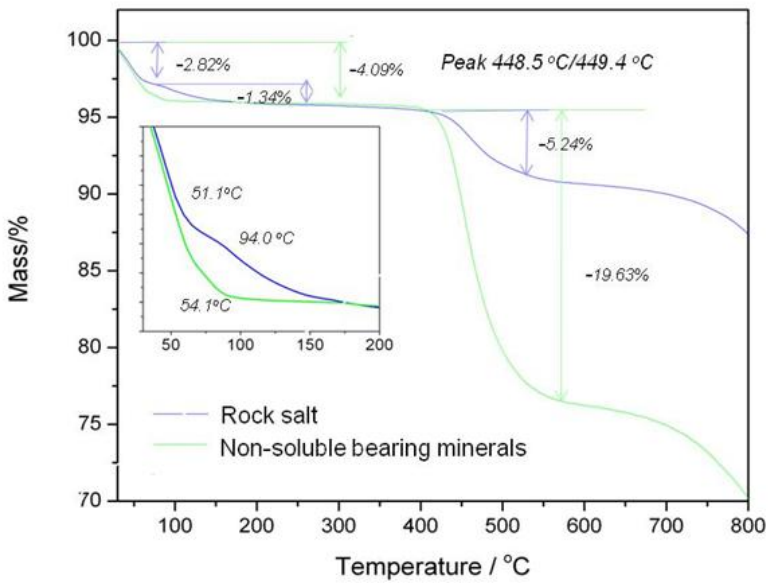
Objective:

Quantify and fingerprint different forms of water in rock salt, and to investigate their mobility under field conditions (T, P) and confinement.

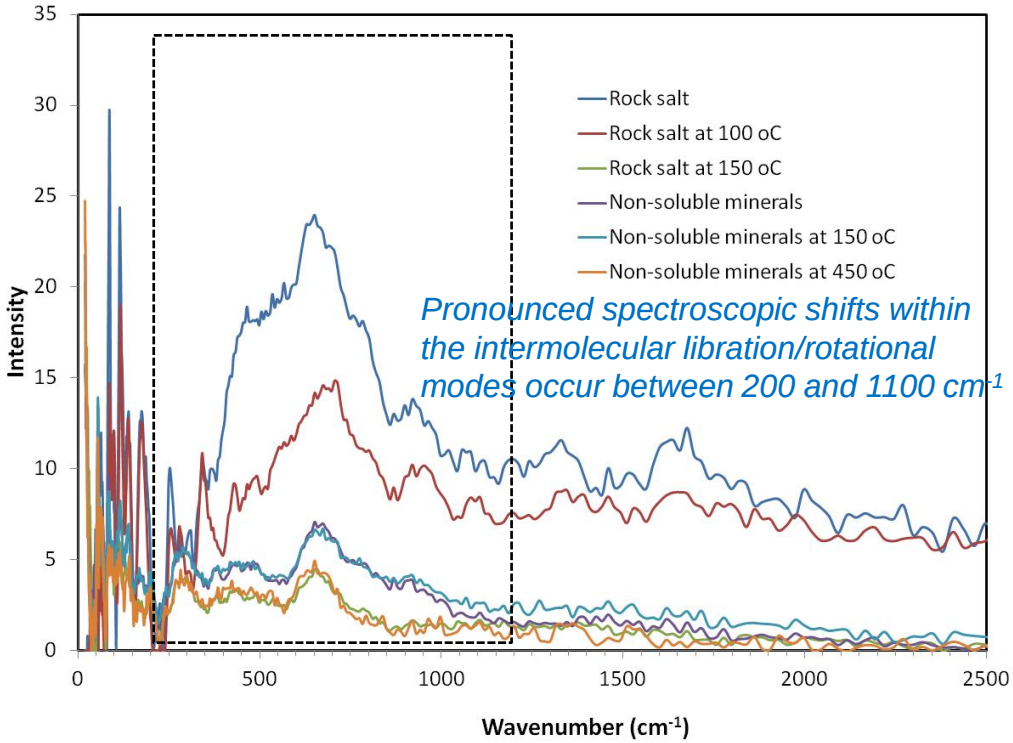
$$f(F\%, B\%, S\%) \Leftrightarrow T, P$$

Confined water and its dynamics in Permian salt

Thermo gravimetric Analysis (TGA)



IINS-FDS spectra



❖ FDS is a vital diagnostic tool for examining confined water behavior in geological material (Ding *et al.*, 2014)

Path-forwards

Capability development

High pressure cell
(P: 45,000 psi; T: 350 ^{o}C)

Pressure fluids flow cell
(under development)

UFD relevance

Fluids flow and transport in low permeability geometrics (e.g., clay, salt) with explicit consideration of pore size, pore network and confinement effects

- Dehydration/swelling
- Elevated P and T
- Flow across heterogeneous geomedia
- Nanoconfined water molecular species and their dynamic behavior

Broad applications and opportunity

- *DOE "Grand Challenges in Subsurface Engineering": SubTER*
- *Experimental investigation thermophysical and chemical properties of fluids flow and transport under pore confinement*