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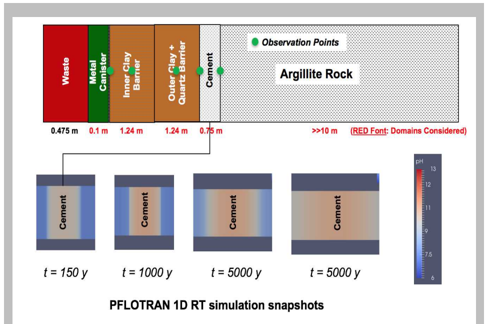
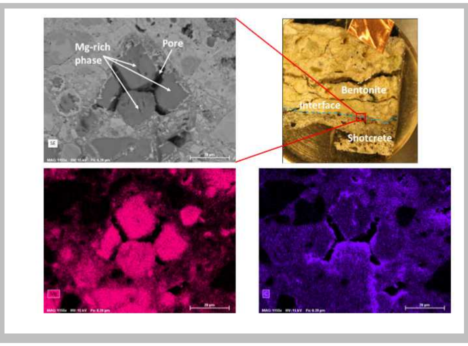


PFLOTRAN 1D RT simulation snapshots



Wasteform Interactions: *Modeling and Advanced Characterization*

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Modelling Approach 1/2

- Based on the experimental program described previously, the simulations will be constructed in an approach that runs parallel to the experimental procedures, as follows:
- Results from rock characterization and liquid-solid partitioning experiments will be used to create 5 rock conceptual models (including mineralogy, porosity, and diffusivity).
- Results from cements characterization and liquid-solid partitioning experiments will be used to create 2 cement conceptual models (including mineralogy, porosity, and diffusivity).

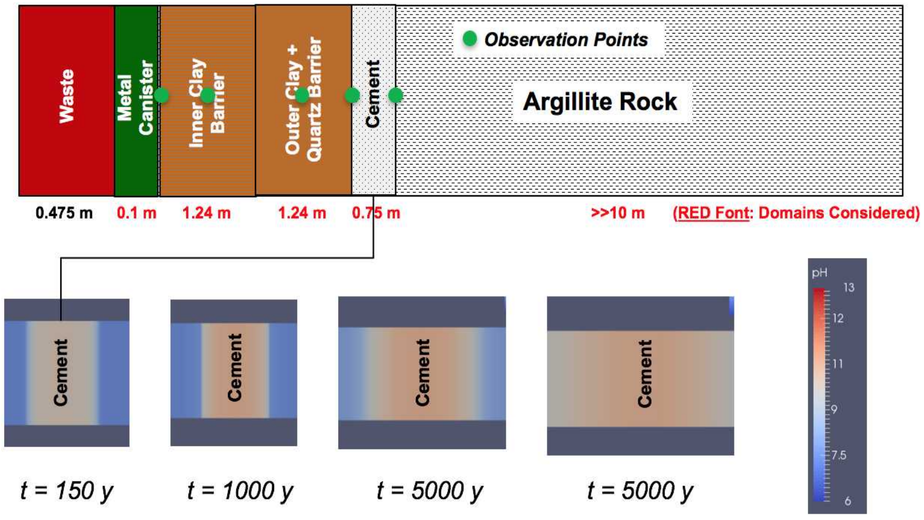
Modelling Approach 2/2

- With the conceptual models complete, reactive transport experiments (results from "infinite bath" testing and rock-cement interface studies) can be simulated. This parallel modelling of experiments can be used to aid the design and/or to aid in interpreting results.
- Benchmarking between LXS and PFLOTRAN and/or EQ3/6 based on laboratory interface test simulations.
- 3D Field–scale PFLOTRAN simulations of cement-rock interactions.

PFLOTRAN Capability

- PFLOTRAN is an
  - open-source,
  - massively parallel,
  - multiphase, 3-D, fully coupled thermos-hydro-chemical (THC) reactive transport code
  - useful for simulating complex multi-phase, multicomponent flow and reactive transport in porous media (Hammond et al., 2014).

- PFLOTRAN also has been used for cementitious materials performance (see figure at right) and environmental assessments.*



PFLOTRAN 1D RT simulation snapshots

For this study, PFLOTRAN code will be applied to diffusive reactive transport in a multi-phase (aqueous and solids) and is more suitable for near-field simulation in complex disposal scenarios (e.g., 2-D and 3-D simulations).

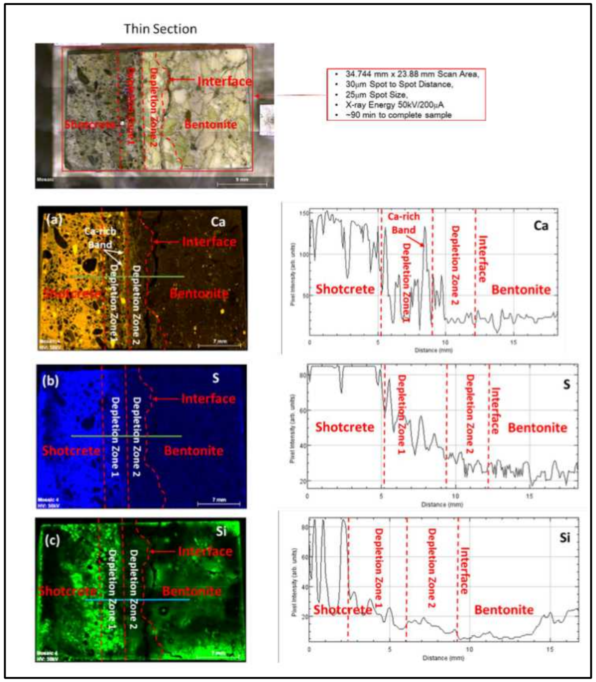
Diffusion Design -> contact intervals

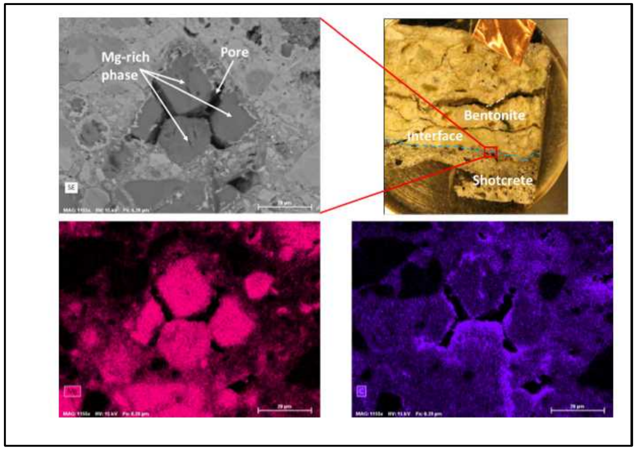
Characterization -> spatial resolution

*Jové-Colón et al. 2016a, Jové-Colón et al. 2016b, Woolery, and Jové-Colón 2016

Advanced Characterization

- Micro-X-ray Fluorescence (μ-XRF) on thin section
- Broad-ion Beam Milling (BIBM)
  - Electron Dispersive Spectroscopy(EDS)
  - Electron Back-Scattered Diffraction
  - Mutli-beam Scanning Electron Microscopy (mSEM)
- Porosimetry
  - Conventional (MIP, N2 adsorption)
  - Advanced techniques using BIBM and mSEM*





* Birkholzer et al. 2017

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