SAND2017-4067PE

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GEOCHEMICAL AND REACTIVE-TRANSPORT EVALUATIONS WITH RELEVANCE TO THE GREET FIELD EXPERIMENT (TASK C)

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U.S. DEPARTMENT OF ENERGY

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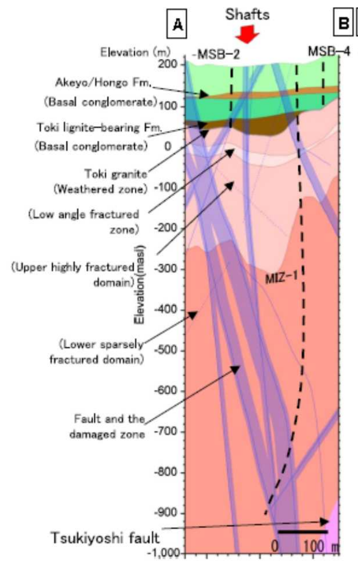
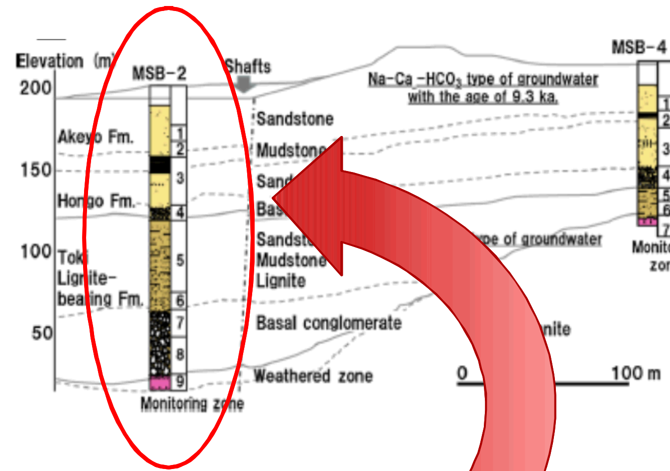
Evaluation of Geochemical Trends in Groundwater Chemistries in Crystalline Rock

- GREET (Groundwater REcovery Experiment in Tunnel)
- Geochemical evaluation of groundwater site data (JAEA GREET website; Iwatsuki et al., 2005 & 2015)

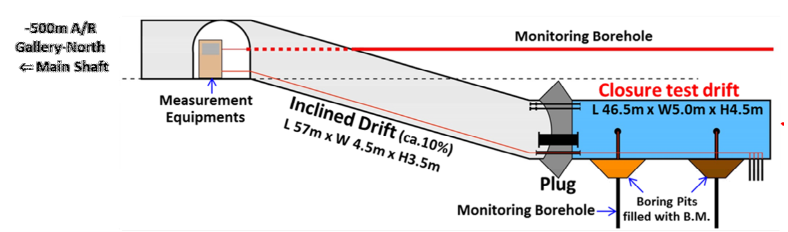




- DECOVALEX-19 Task C:
  - **Current focus: geochemical evaluation of groundwater chemistry trends**
  - Evaluation of monitoring hydrological and geochemical site data (e.g., Closure Test Drift - CTD)
  - Interactions with host-rock and barrier materials

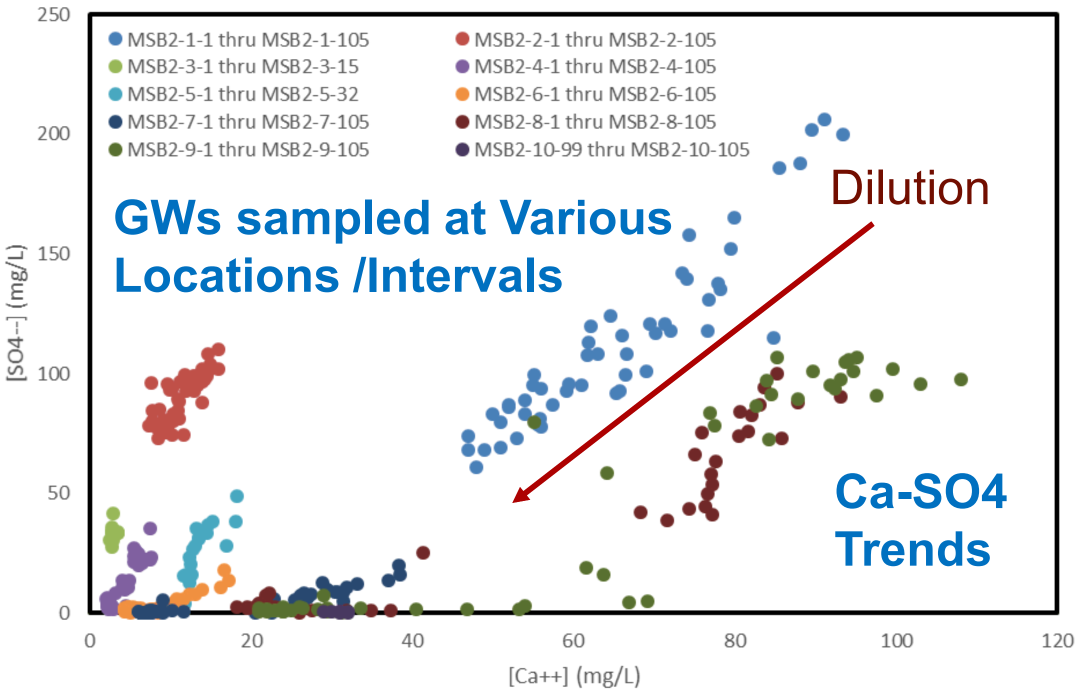
Monitoring Borehole MSB-2 Evaluation

Closure Test Drift - CTD



GREET: Groundwater Chemistry Site Data

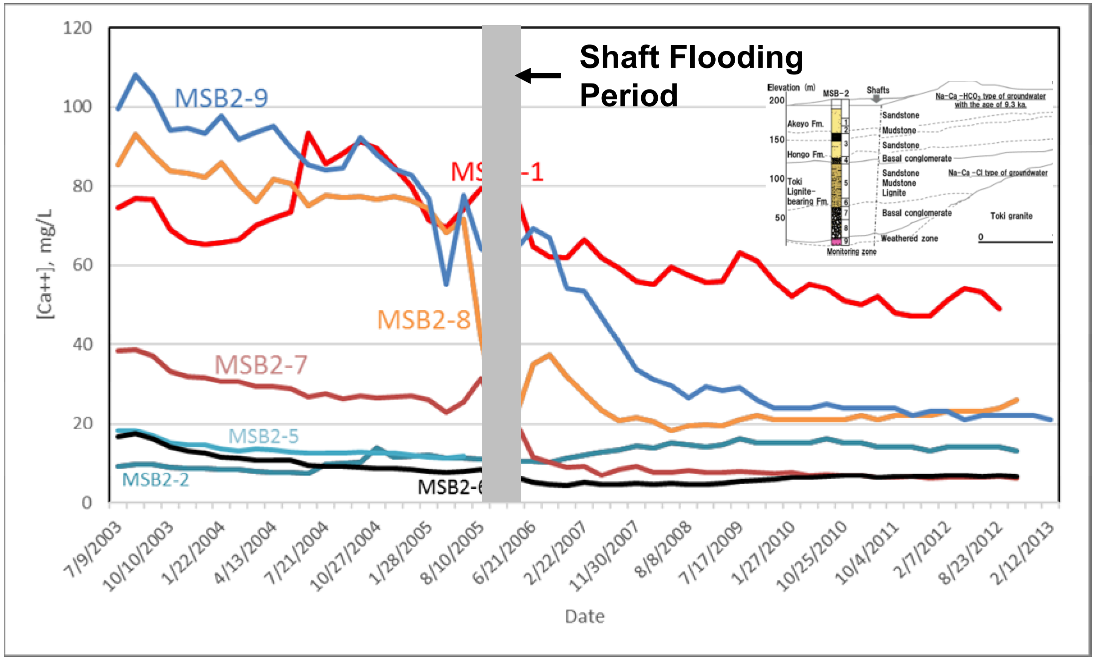
MSB2 Monitoring Borehole Total Data (Ca & SO_4)



- Dilution → Overall, applies to major constituents:
  - Ca, SO_4, K, Na
- Trend variations in different zones
  - e.g., Na, Cl concentrates in certain zones

- Evaluate geochemical trends:
  - Time -> Separate flood event
  - Location -> Spatial correlation for chemical trends
- Geochemical modeling
  - EQ3/6 code simulations
    - Reaction path modeling (dilution, mixing)
    - Aqueous speciation
      - Charge imbalances
      - GW chemical evolution
    - GW saturation state
    - Mineralogic interactions

GREET: Groundwater Chemistry Site Data: MSB2 monitoring borehole



- Evaluate geochemical trends:
  - Time -> Separate trends from flood event
  - Zones -> Spatial fluid mixing between zones
- Geochemical modeling
  - EQ3/6 code simulations
    - Reaction path modeling
      - Pure water dilution of MSB2-1 analysis
      - Mixing of waters from different zones (mixing MSB2-7 with MSB2-1 groundwater)
      - No mineral saturation considered
    - Geochemical speciation
      - Assess bicarbonate concentrations
      - Charge balancing

Goals:

- Explore evaluation of groundwater mixing in boreholes using geochemical modeling
- Assess application of geochemical tools to predict groundwater chemistry

GREET: Groundwater Chemistry Site Data: MSB2 monitoring borehole

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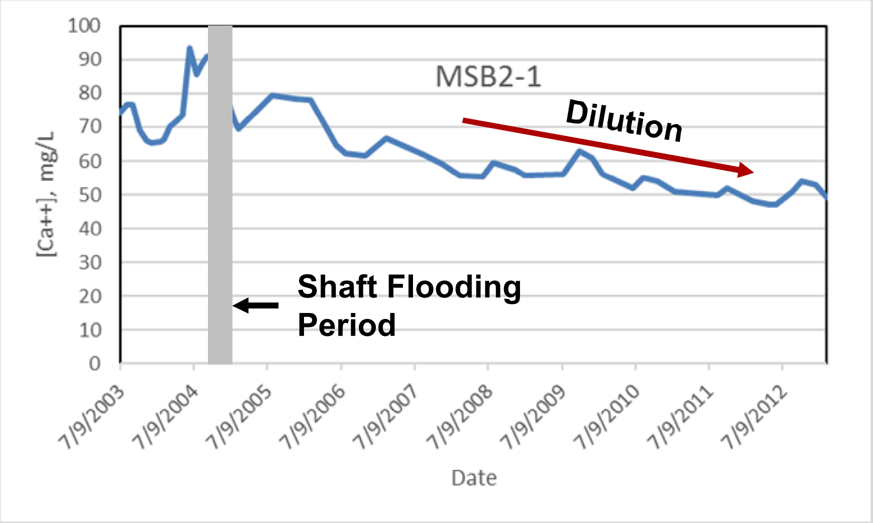
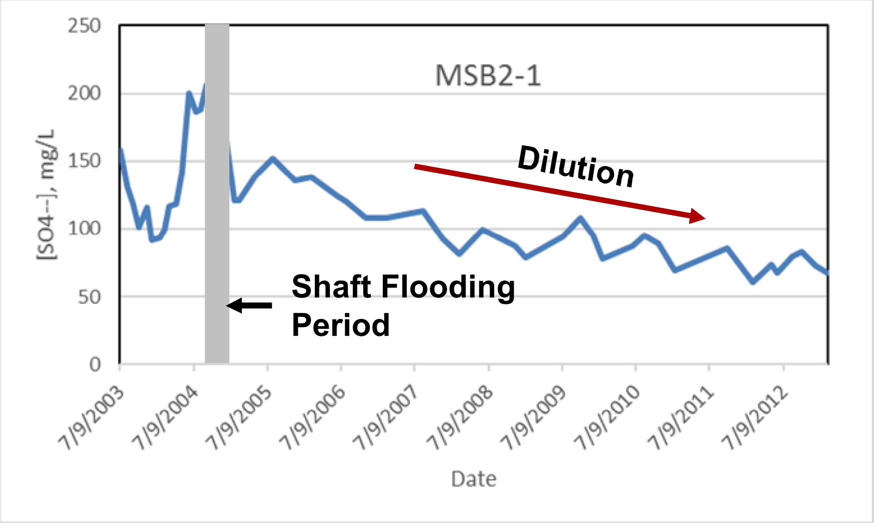
MSB2 Monitoring Borehole Zone 1: Dilution with time





GW mixing Modeling:

- [Ca^{++}] and [SO_4^{--}] selected as dilution indicators
- Only post shaft flooding GW composition considered
  - Large variations in pre shaft-flooding data
  - Only data showing progressive dilution trends
- Other aqueous species will be considered in subsequent evaluations

GREET: EQ3/6 GW mixing Simulation: MSB-2 monitoring borehole (Zones 1 & 7)

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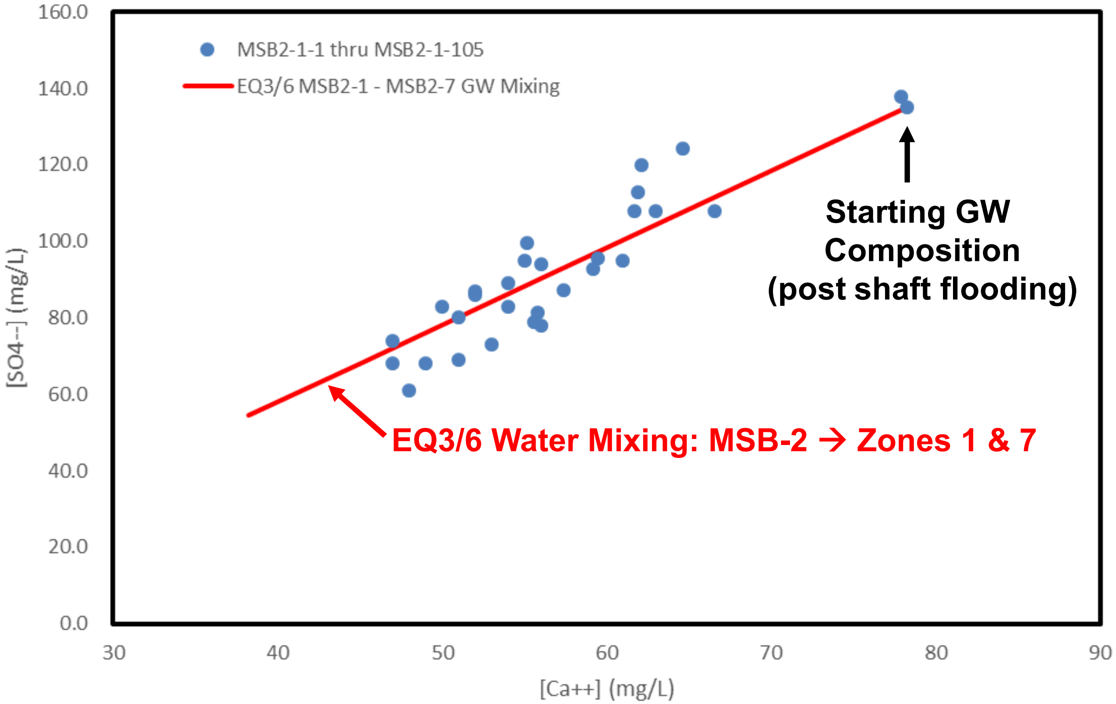


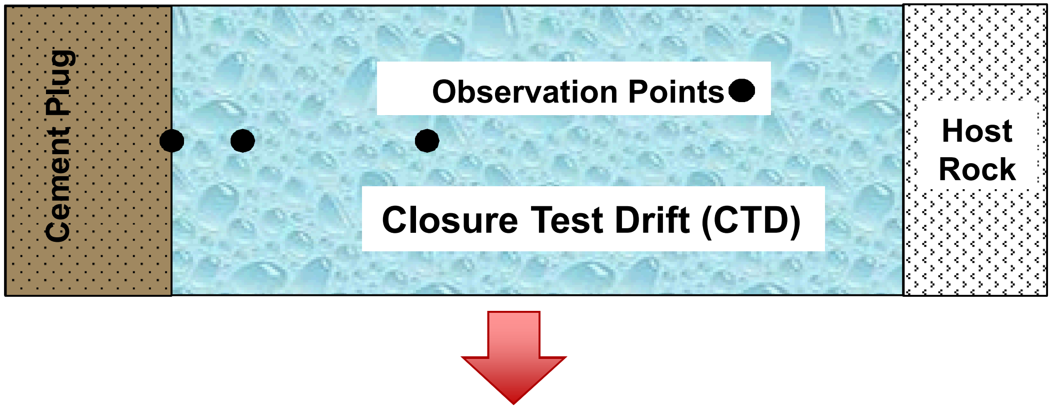
TODO Next:

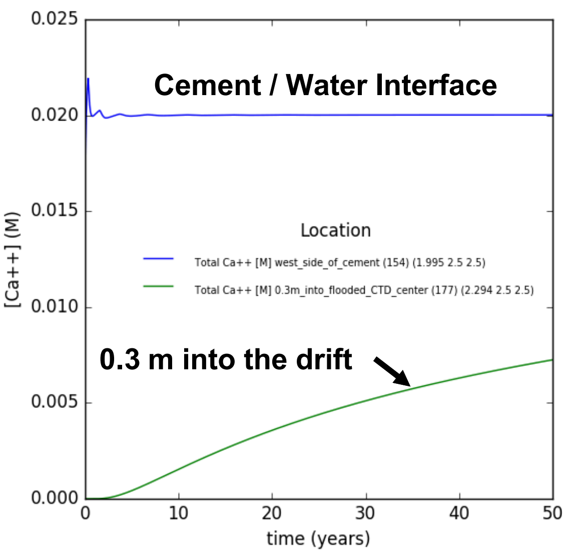
- Consider different starting GW compositions: MSB2-1 & MSB2-4
- Consider other GW chemistries: MSB4, WR's, Galleries
- Simulate mineral saturation effects: e.g., calcite

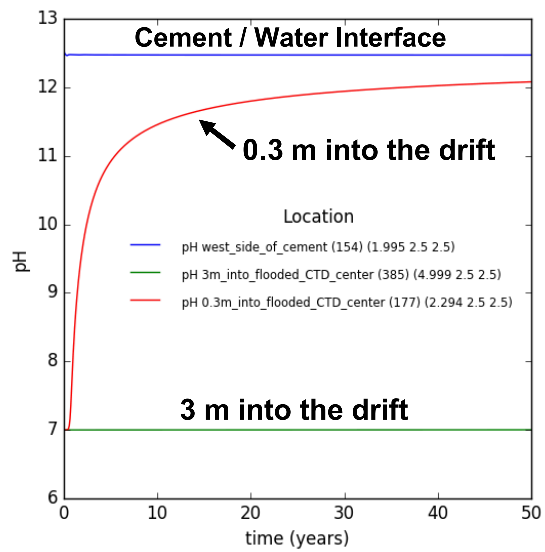
- Evaluate dilution trends:
  - EQ3/6 simulation of MSB-2 GW mixing of Zones 1 & 7
  - Test flood water provenance: likely from MSB-2, Zones 7 & 8 (Iwatsuki et al. 2015)
- Simulation Results
  - Ca vs SO_4 dilution trend is represented by the GW mixing for MSB-2, Zones 1 & 7
  - Simulation predicts increases in [Na] & [Cl] as observed but at higher concentrations
  - Assess discrepancies in predicted trends
    - Fresh water input?
    - Mixing with a more dilute water?

Closure Test Drift (CTD): H-C Model

PFLOTRAN 1D Reactive Transport Modeling







- H-C (Reactive-transport - RT) modeling
  - **PFLOTRAN** RT simulation tool
  - 1D reactive-transport model
    - Cement plug / CTD region
    - Flooded CTD region modeled as a high porosity / high permeability domain
    - Diffusion only
    - OPC cement composition
    - Diluted “fresh” water composition in flooded domain
    - THERMODDEM thermodynamic database including cement phases
  - Effects of cement interactions on bulk water chemistry
    - As expected, large changes in pore & bulk fluid composition at the vicinity of the cement / water interface (see Figs.)
    - Increases in Ca & pH can be significant even at 30 cm from the interface
    - Next: Sensitivity analyses on transport parameters, kinetic rates, aqueous species profiles