UDC contribution to Working Group 3: High temperature clay interactions

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UDC presentation

- **University of A Coruña: UDC**
  - One of the 3 universities of Galice (Northwest Spain)
  - Created in 1990

- **Reactive Transport Group** @ Civil Engineering School
  - The group is strong on THC(m) numerical modeling
  - 30 years of expertise

UDC general expertise

- **Main model capabilities/features**
  - Coupled water flow, heat transport & multicomponent reactive transport of chemical species and radionuclides
  - Comprehensive and general conditions:
    - Saturated/unsaturated, homogeneous/heterogeneous, isotropic/anisotropic
  - Single or multi-phase non-isothermal flow conditions
  - Porous and fractured media
  - Simultaneously geochemical & microbial processes
  - Geochemical reactions: aq. complexation, acid-base, redox, cation exchange, surface complexation & mineral dissolution/precipitation (LEA & kinetics)
  - Single/dual porosity
- **In-house computer codes**
  - CORE series (CORE; INVERSE-FADES-CORE)

UDC general expertise

EC research projects

- Since 1991
- Clay & bentonites
  - CERBERUS
  - FEBEX I, II
- Near field
  - NFPRO
  - **PEBS**
  - **CEBAMA**
- Far field
  - FUNMIG
- Performance assessment
  - BENIPA
  - PAMINA

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UDC general expertise

EC research projects

- Since 1991
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Projects funded by ENRESA

- Since 1987
- Radwaste facilities
  - Interim Storage facility
  - Uranium mill tailings
  - El Cabril LLW repository
- Transport models for Clays
  - Spanish Clay
  - DI-B experiment in Opalinus clay (Mont Terri)
- Natural Analogues
- Performance assessment
  - ENRESA 2000 (granite)
  - ENRESA 2003 (clay)

UDC general expertise

Other WMO's

- SKB
  - Microbial processes
  - Redox Zone
  - Concrete degradation
- ANDRA
  - DIR experiments
- NAGRA - Mont Terri
  - DR experiment

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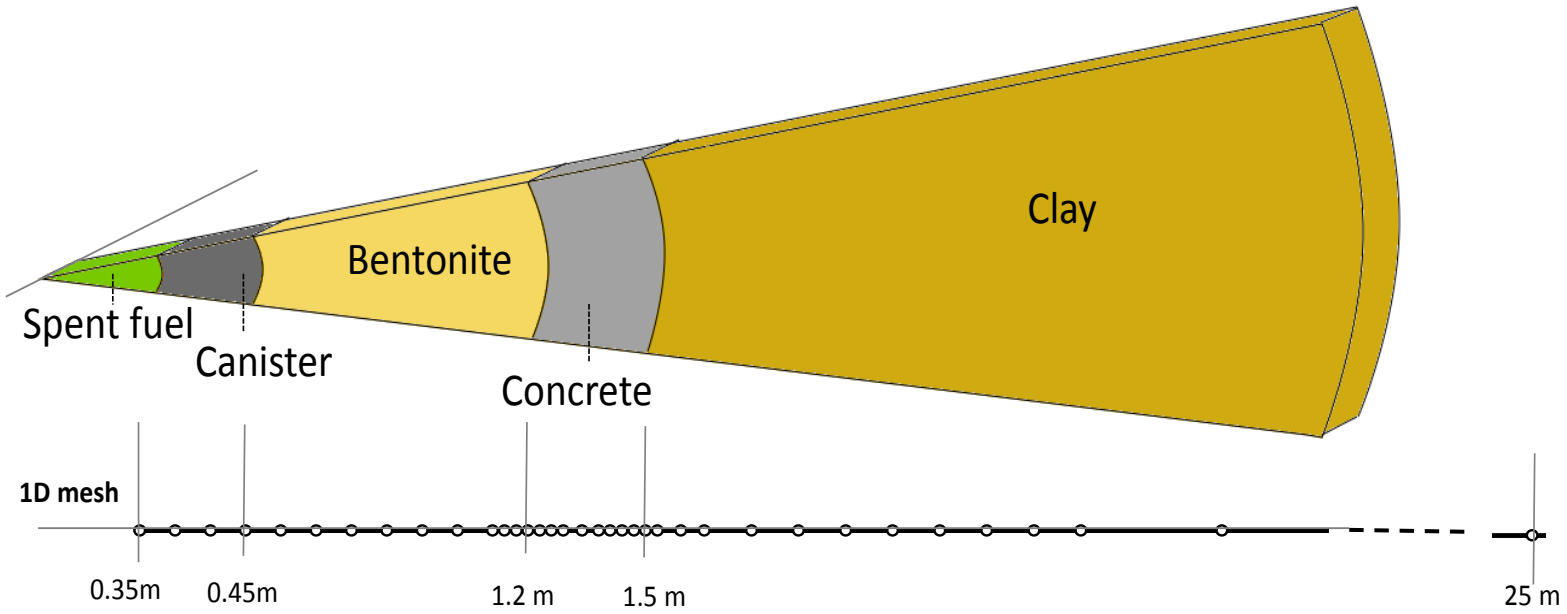
UDC specific expertise for WG3

- Most recent research of UDC related to the tasks of **High Temperature Clay Interactions**
  - Long-term simulations of the interactions of compacted bentonite, concrete and carbon steel in a repository in clay (PEBS Project)



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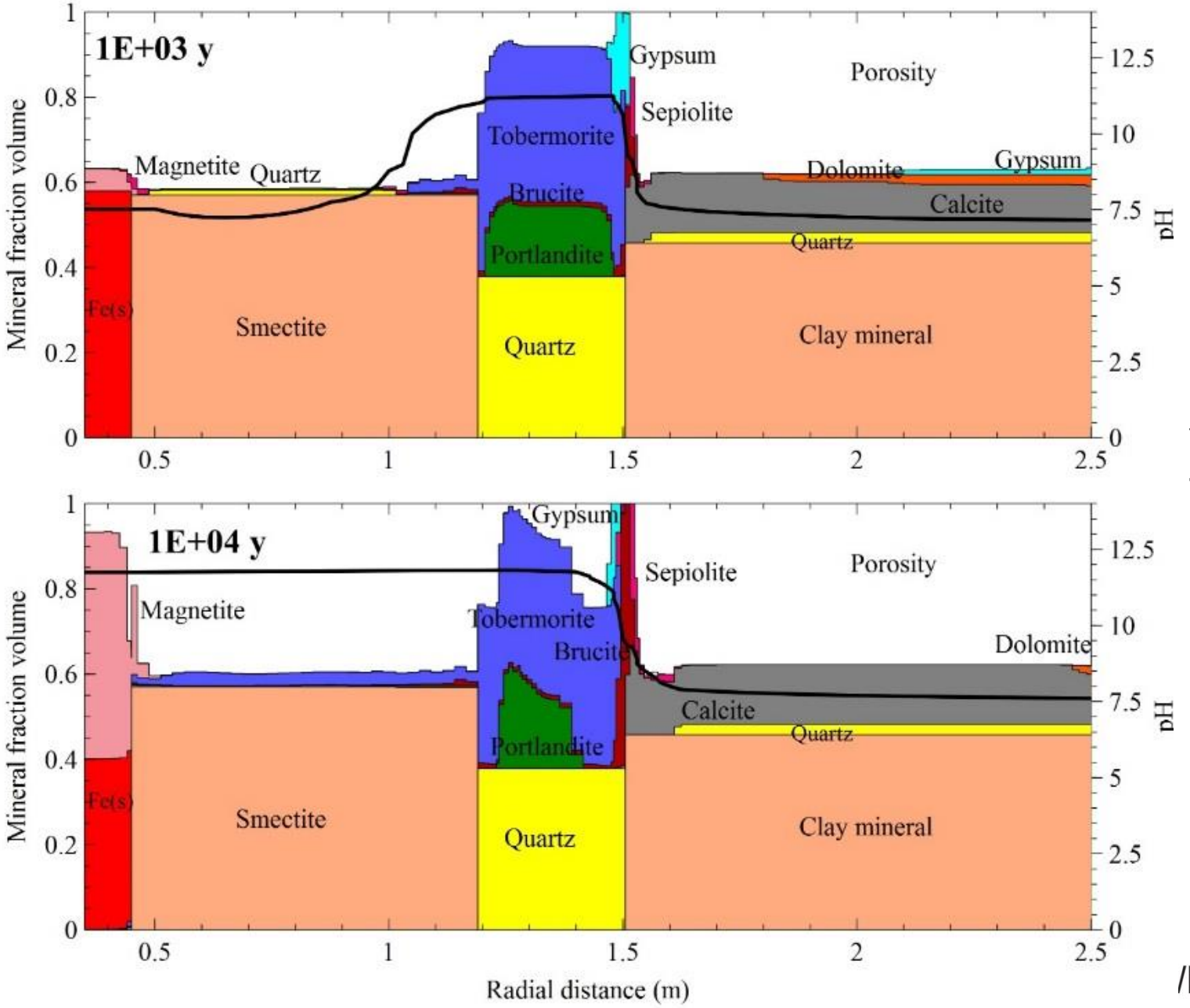
UDC specific expertise for WG3



Interactions of corrosion products, bentonite & concrete: volume fractions of minerals and pH

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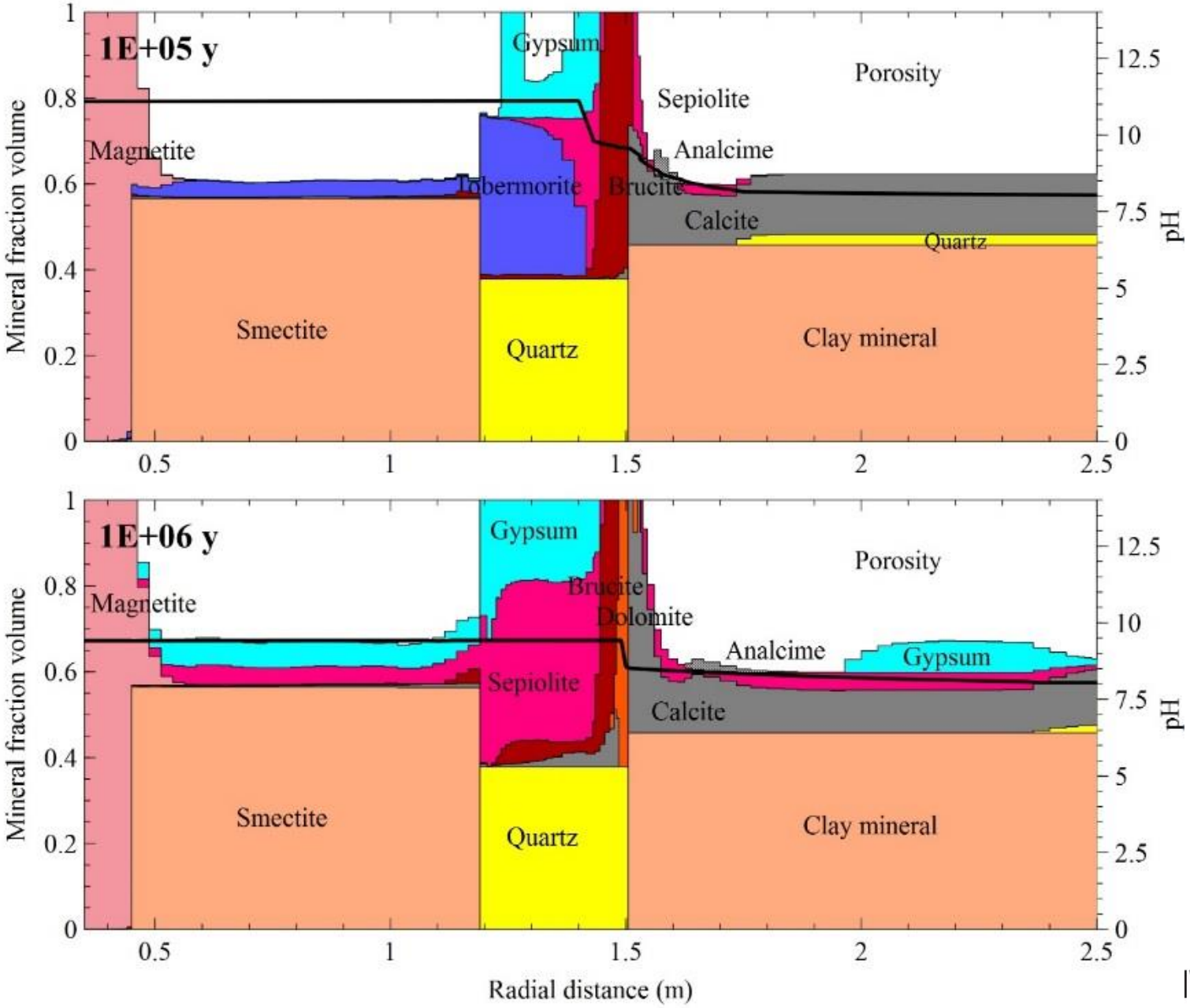
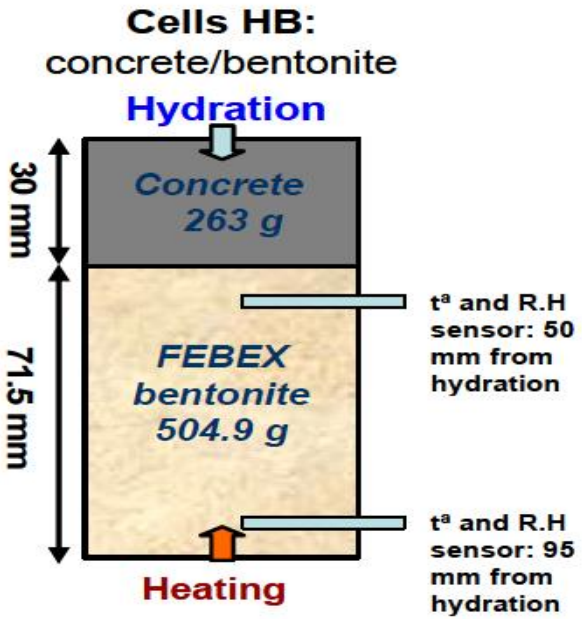
UDC specific expertise for WG3

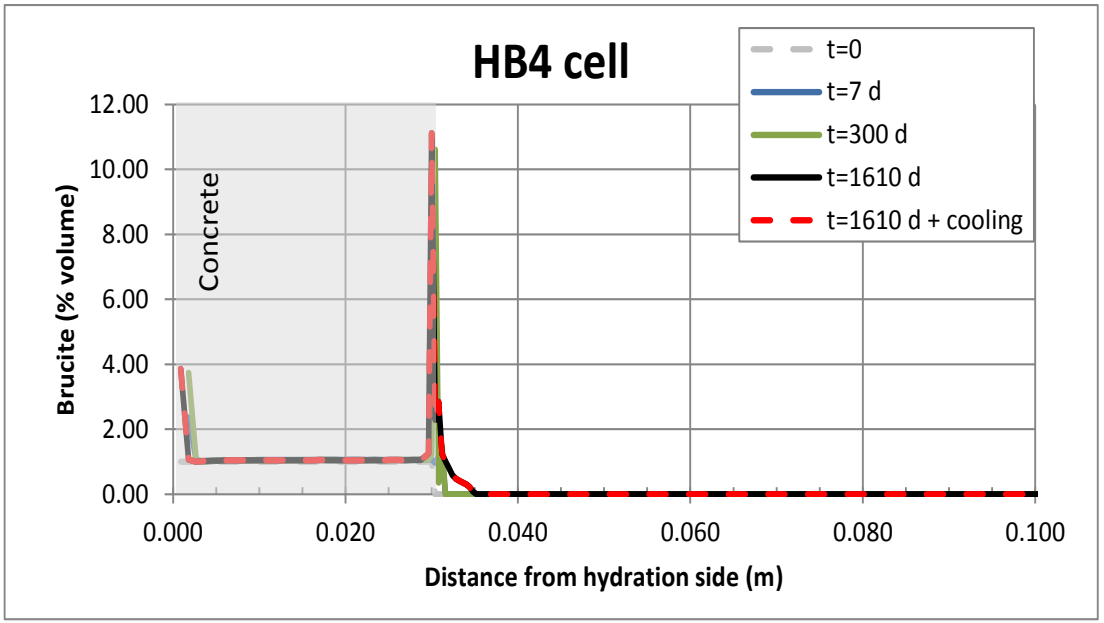


Interactions of corrosion products, bentonite & concrete: volume fractions of minerals and pH

UDC specific expertise for WG3

- Most recent research of UDC related to the tasks of **High Temperature Clay Interactions**
  - THCm models of heating (100º C) and hydration tests. Interactions of compacted bentonite with concrete performed by CIEMAT-UAM (CEBAMA Project, 20015-2019)





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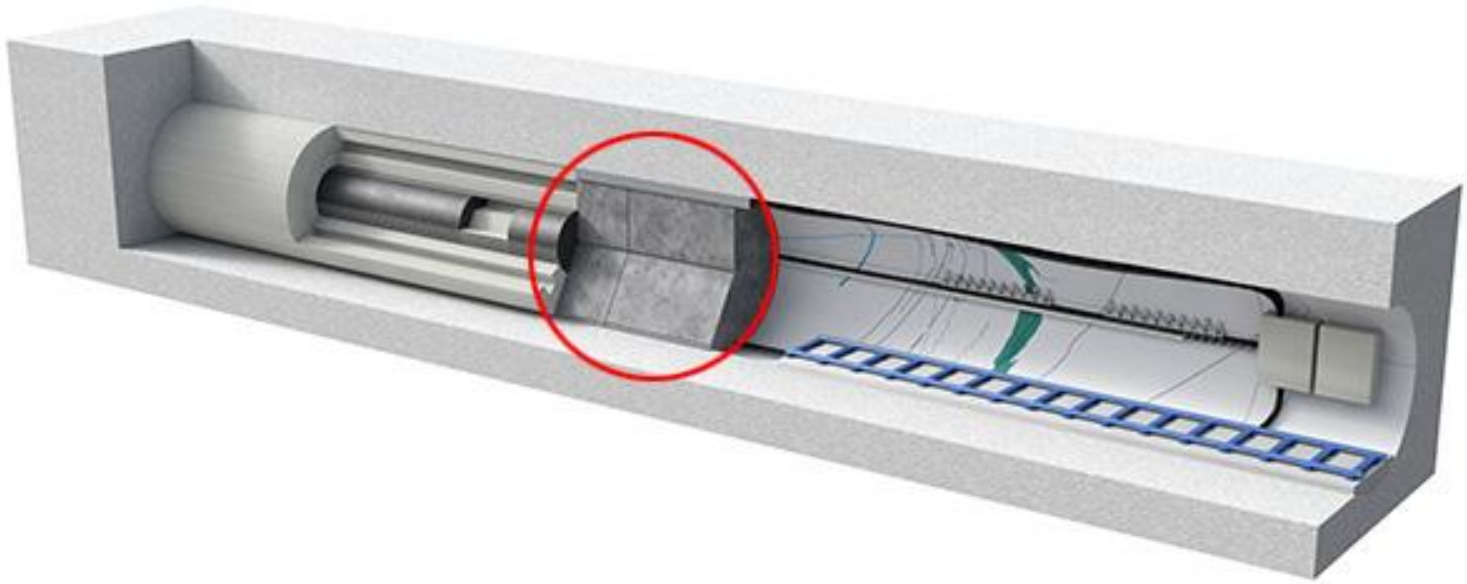
UDC specific expertise for WG3

- Process understanding and model capabilities have been developed from previous Projects such as FEBEX & FEBEX-DP
- FEBEX in situ test at the Grimsel Test site:
  - Heating (100ºC) and hydration test.
  - Full scale of the EBS: 1997-2015



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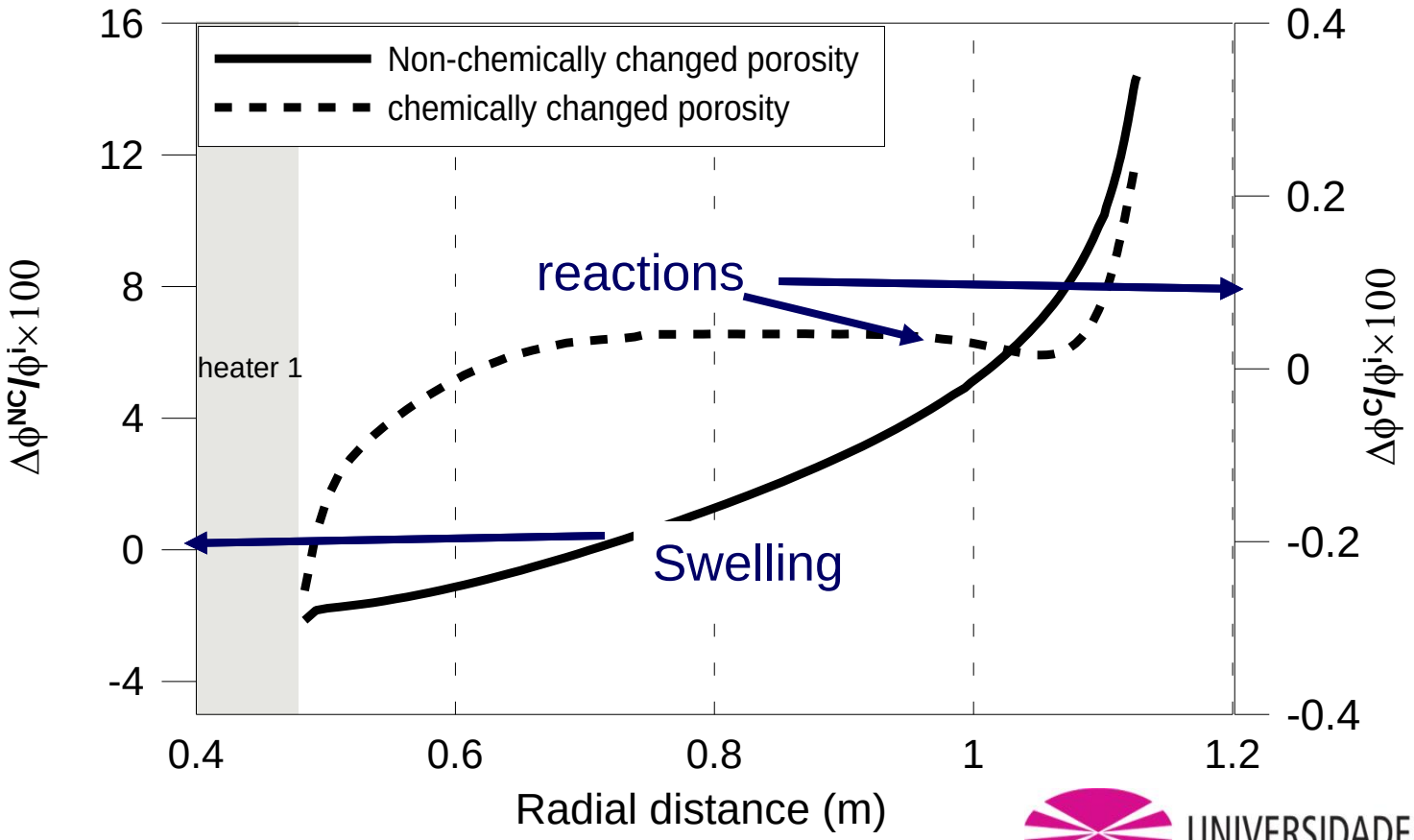
UDC specific expertise for WG3

- Process understanding and model capabilities have been developed from previous Projects such as FEBEX & FEBEX-DP
- Computed changes in porosity
  - Swelling (Non Chemical)
  - Mineral dissolution/precipitation (Chemical)



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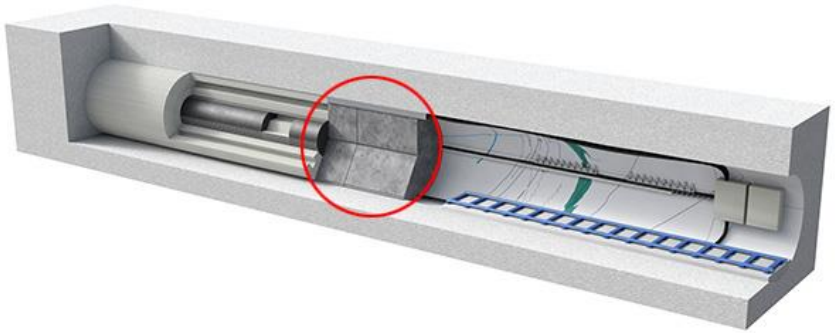
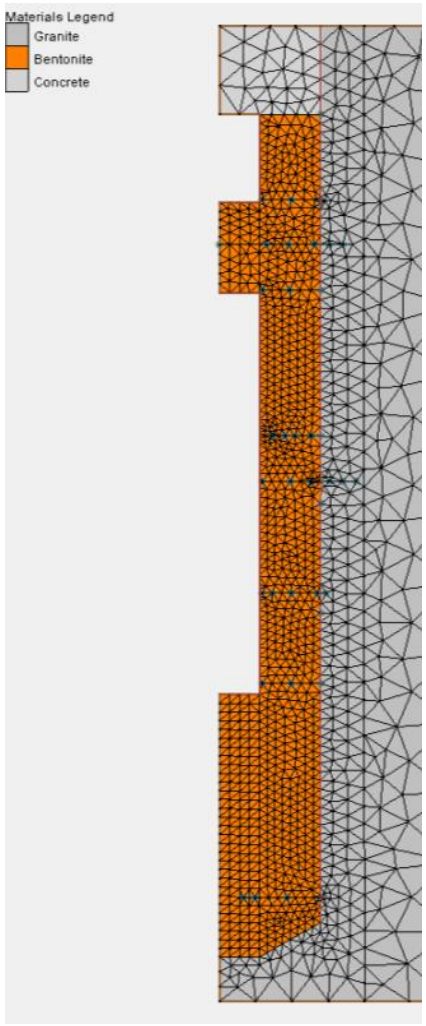
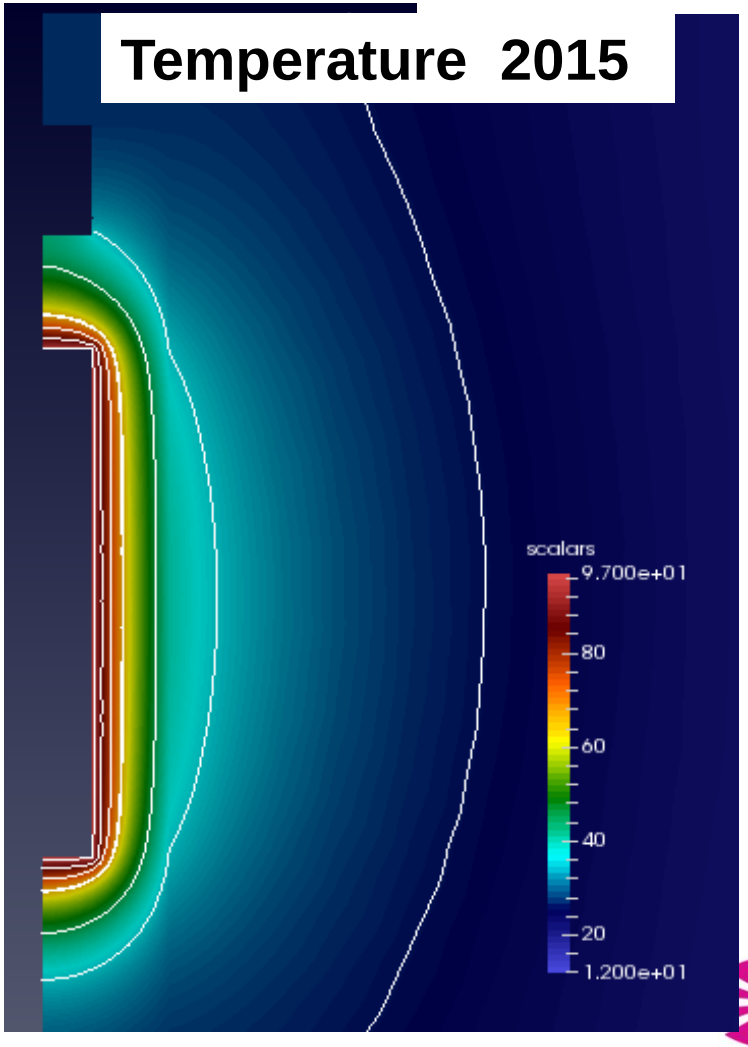
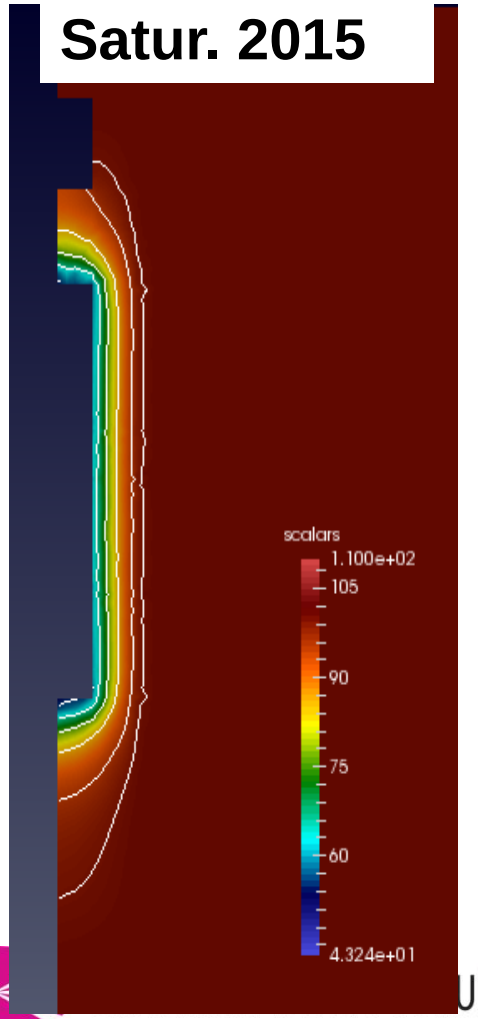
– FEBEX-DP: Temperature & saturation degree predictions after 18 years of heating and hydration

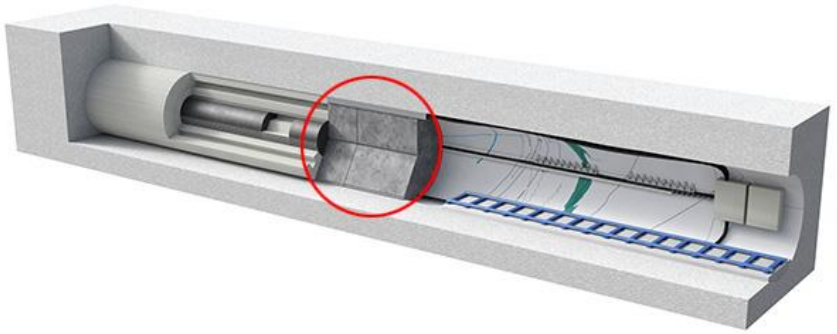


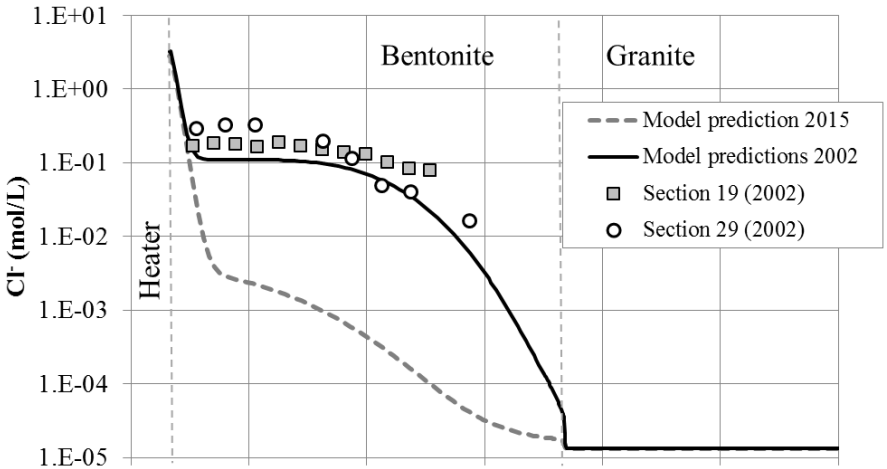


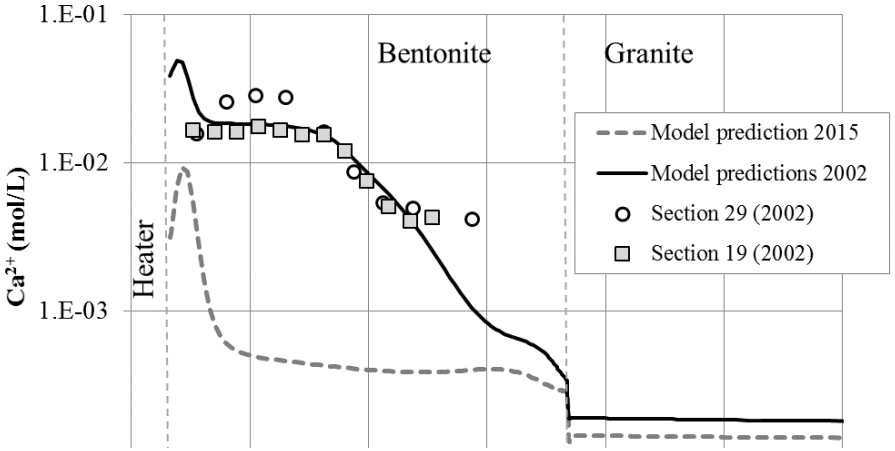


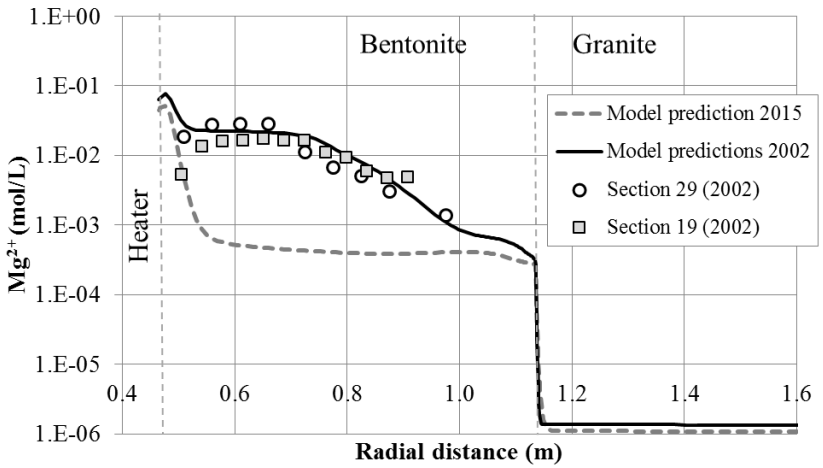


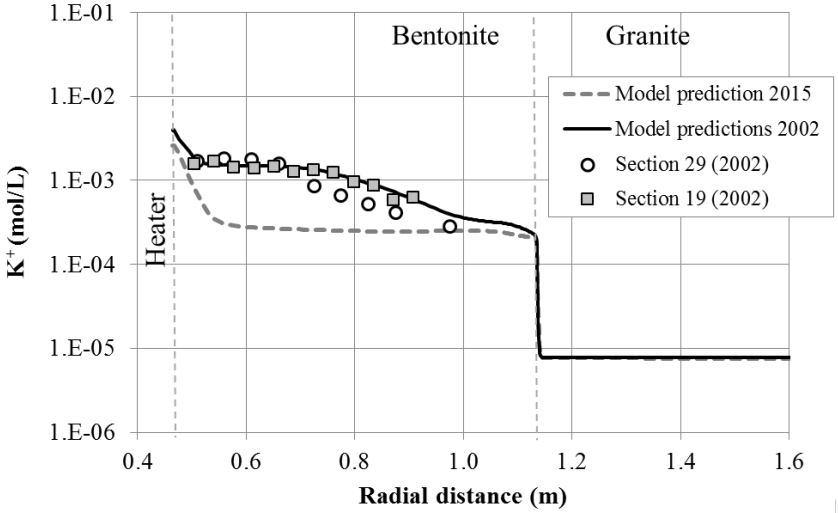
– FEBEX-DP: THC predictions of the chemical conditions after 18 years of heating and hydration











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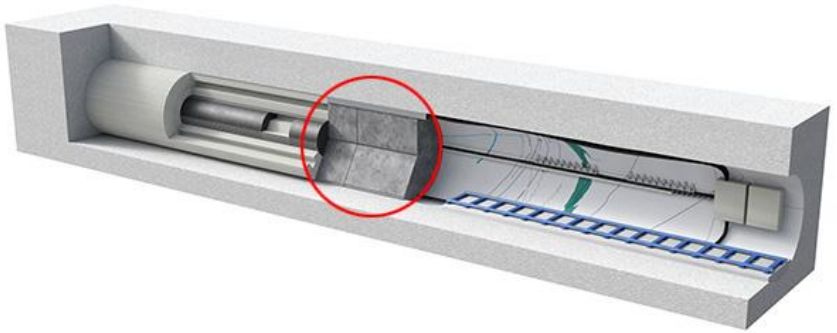

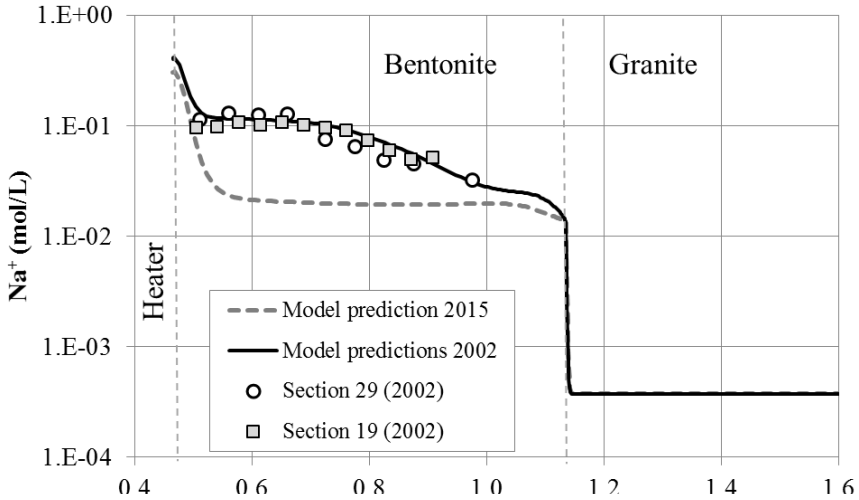

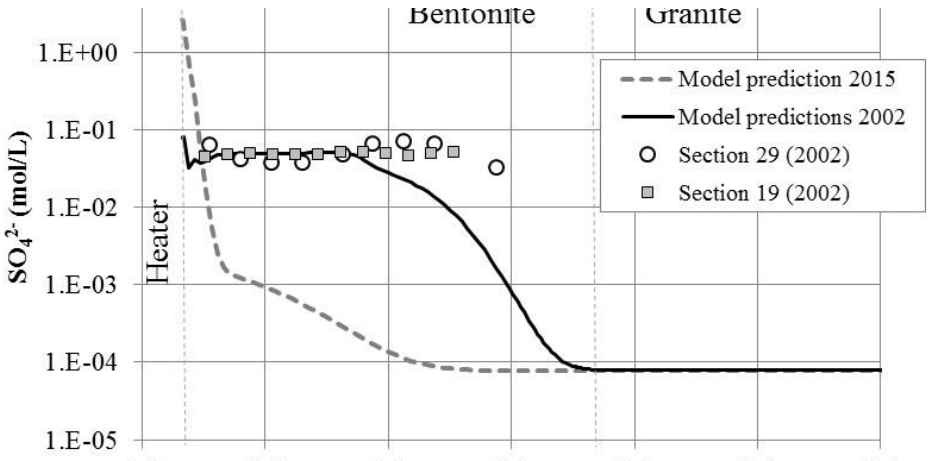

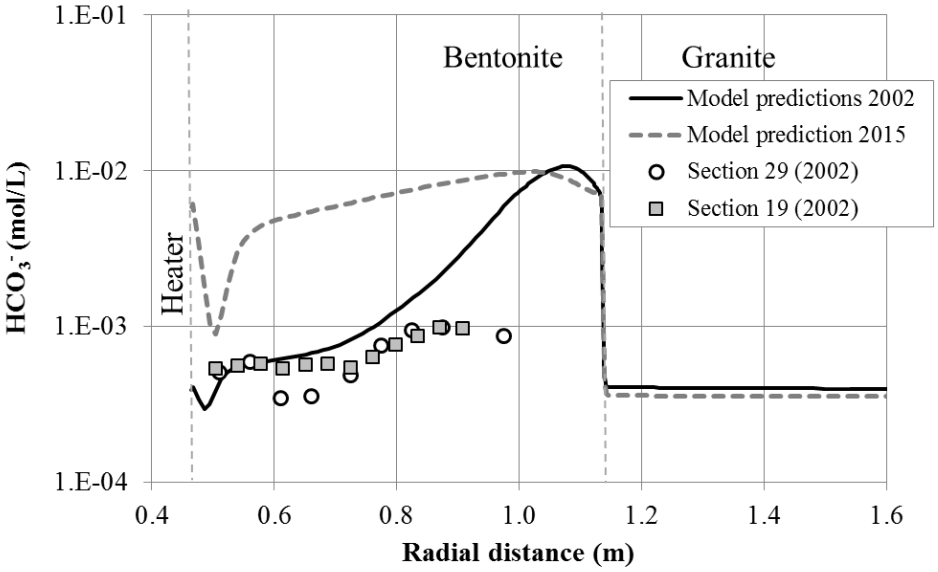

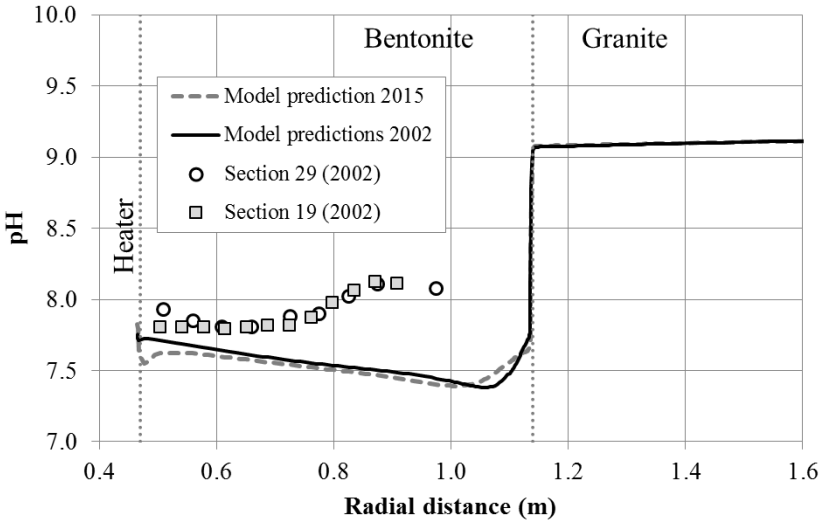

UDC contribution to Working Group 3

- **Background on high T clay interactions**
  - High temperatures enhance illitization & cementation in the bentonite buffer and the clay formation
  - Illitization: smectite to illite transformation

$$smectite + K^{+} (+ Al^{3+}) \rightarrow illite + SiO_2 + (Ca, Na)$$

  - Complex slow kinetic conversion process which depends on T, K activity, pressure, smectite mineralogy, dissolved and and exchanged cations, water activity, solute transport, & chemical factors such as the concentrations of Al and the dissolution rate of clay minerals
    - Multicomponent reactive transport THC models are needed
  - Key factors: high temperatures and large K activities

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UDC contribution to Working Group 3

- **Background on high T clay interactions**
  - Potassium:
    - Potential sources: dissolved K in the clay formation, dissolution of K-feldspars, exchanged K in the interlayer & cement materials
    - Slow diffusion may limit illitization
  - Decrease in smectite content may decrease the swelling stress and the retention capacity of the EBS bentonite
  - Higher temperatures lead to much higher evaporation rates, vapor pressure buildup in the EBS bentonite and clay host rock, and mineral precipitation (cementation)

UDC contribution to Working Group 3

- **Background on high T clay interactions**
  - Lack of adequate experimental data and natural analogues representing the conditions of the buffer and host rock of SF/HLW repositories
  - Need to integrate the relevant THMC processes and consider the interactions of the EBS and the host rock
- **Motivation & Purpose**
  - The assessment of the impact of increased temperatures on the buffer performance and properties requires the scientific understanding of the underlying processes at higher temperatures and the use of well-established and verified THM and THC numerical models and codes

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UDC contribution to Working Group 3

- **Contributions**
  - Extending and improving the current THCM models and codes
    - Modelling of illitization
    - Handling extremely large concentrations near the heater
    - Including the chemical changes at the canister-bentonite interface
      - The release of Fe might enhance the dissolution of smectite by precipitating Fe phyllosilicates
    - Improving the couplings of chemistry to mechanics
  - Benchmarking of the coupled THCM code
  - Modelling high temperature lab and in situ tests (such as HotBENT)
    - Design stage (dimensions, location of sensors, …)
    - The interpretation of the actual experimental data
    - THCM model of hot-FEBEX: compare results and performance of FEBEX (100ºC) and hot-FEBEX (150 to 200ºC)
  - Modelling the long-term geochemical effects of the high temperatures

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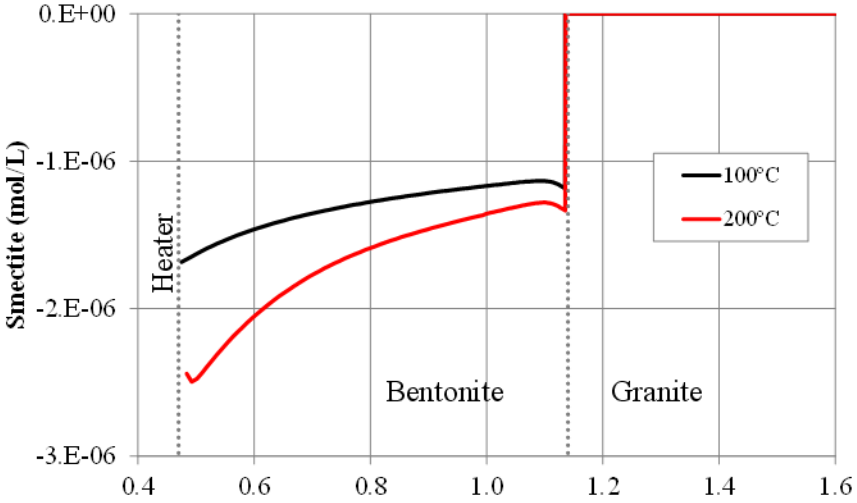
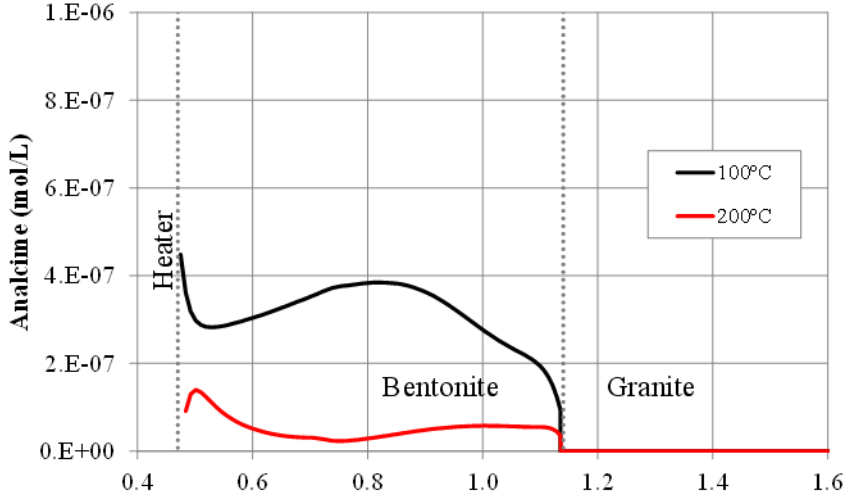
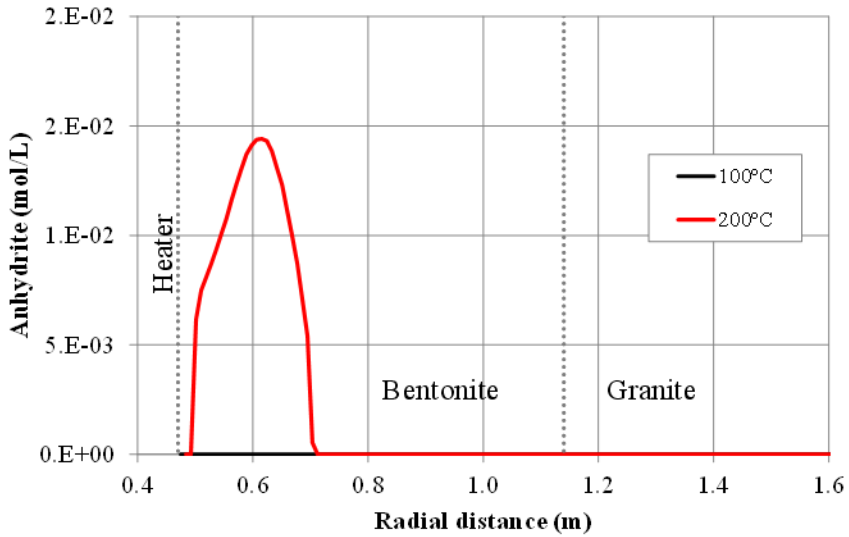
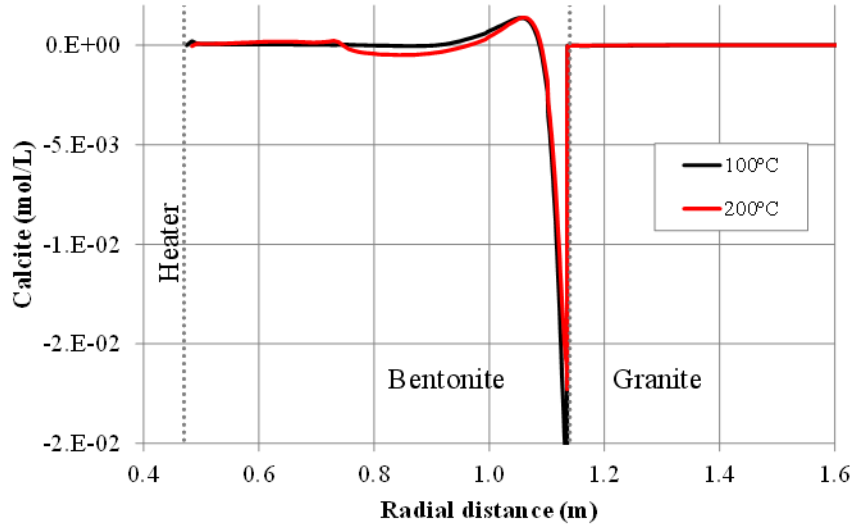
UDC contribution to Working Group 3

- **Contributions**
  - Some preliminary results: smectite dissolution & analcime prec. for FEBEX in situ test at 2002









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UDC contribution to Working Group 3

- **Issues that should be resolved**
  - Evaluate the effects of high temperatures on bentonite and host rock properties such as porosity, swelling pressure, CEC
  - The changes in porosity will affect flow and mass transport parameters
- **Integration with other teams**
  - Modelling lab and in situ experiments
  - Code benchmarking
  - Inter-comparison of predictions for different bentonites
- **Resources needed**
  - PhD Student (3 years)
  - Traveling costs
  - PhD advisor (6 months)
  - Indirect Costs (25%)

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