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# Numerical Modelling and Repository Design:

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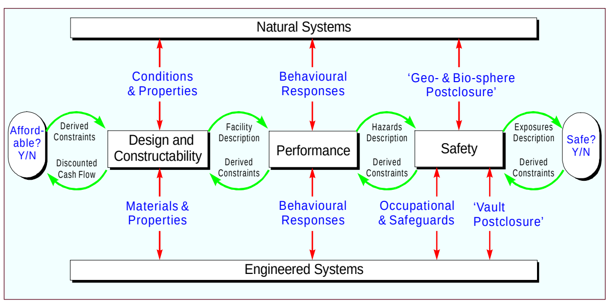
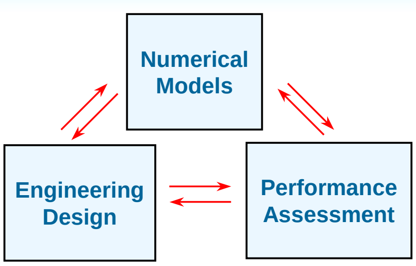
## The Process for Repository Engineering






## Role of Numerical Models




Specific numerical models for material response and various physical processes models are required for support of both engineering design and performance assessment

## Numerical Models for Materials & Processes

- **Provide direct input to performance assessment**
- **Confirm appropriateness of simplified performance assessment models**
- **Understand important phenomena that might affect system performance**
- **Develop design criteria for construction and engineered barriers**
- **Provide means for correlating single-point measured responses (i.e., pore pressure, displacement, acoustic emission) from monitoring instrumentation with possible events occurring within a sealing system**



## Numerical Models for Repository Design

Repository designers use numerical models to ensure that specific design criteria are achieved and that safety to the public and workers is assured. Repository design requirements may include:

- Minimizing rock damage around openings
- Minimizing potential for fracturing in the rock
- Ensuring integrity of backfill under container loads
- Ensuring low permeability of backfill under hydraulic and thermal loads
- Ensuring construction interfaces (e.g., between backfill and rock) are not preferred hydraulic pathways
- Ensuring that engineered barrier materials (clay, concrete grout) perform as required over the long-term



## What Should be Modelled?

**Laboratory tests**

- **Well-controlled conditions**
- **Good for developing fundamental process models**

***In-situ* tests**

- **Representative of *in-situ* materials and conditions**
- **Demonstrate that models are both appropriate and applicable to expected repository conditions**

## Importance of Modelling *In-situ* Experiments

**Confirm that models apply:**

- **At full-scale**
- **Under representative boundary conditions**
- **Using materials that are undisturbed by sample retrieval**
- **Using rock that is representative of *in-situ* rock (*in-situ* fracture properties, representative damage as induced by excavation)**

**The results from lab tests may be very different from field tests**

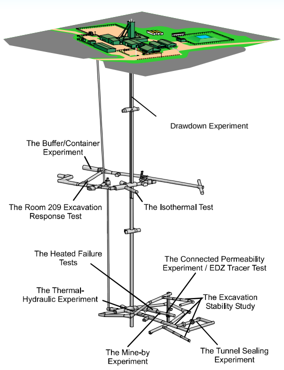


## *In-Situ* Experiments

- **AECL has used the Underground Research Laboratory (URL) to perform *in-situ* experiments in a representative geologic setting in support of design and performance assessment of a deep geologic repository.**
- **All experiments at the URL have numerical modelling components**



## URL Experiments



## Forward Prediction and Back Analysis

Forward predictions for model validation are often a requirement of experimental programs

Difficulties in using *in-situ* experiments for model validation include:

- Lack of pre-established criteria for success of model validation (difficult to predefine criteria)
- Experiments are not well suited to test models (result in ambiguous comparisons)
- Back-analysis not performed (discrepancies between measurement and prediction unresolved)
- Boundary conditions and *in-situ* material properties not sufficiently well defined for experiment



## Forward Prediction and Back-Analysis

Forward predictions are important to demonstrate understanding of relevant processes

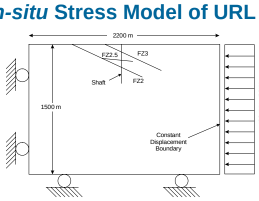
An important lesson learned from the URL -

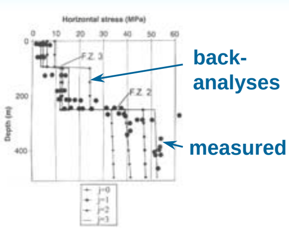
Back-analysis of experimental data is at least as important as forward prediction in learning what may have occurred in the experiment so that this knowledge can be demonstrated in future tests and applied to repository design/performance assessment



## Useful Example of Back-Analysis

*In-situ* Stress Model of URL

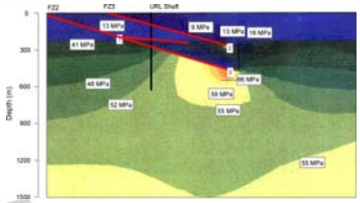


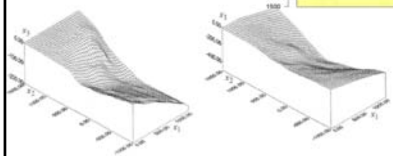




By matching computed stresses with measured *in-situ* stresses, information on far-field stress conditions, *in-situ* rock modulus and fault shear displacement properties can be obtained. Prediction of stress at depth before taking measurements would have been unsuccessful.

## Back-analysis of URL *In-situ* Stress Model

Computed stress was strongly affected by proximity to faults and fault properties





Back-analysis was improved by using a 3-D model with a 3-D fault geometry



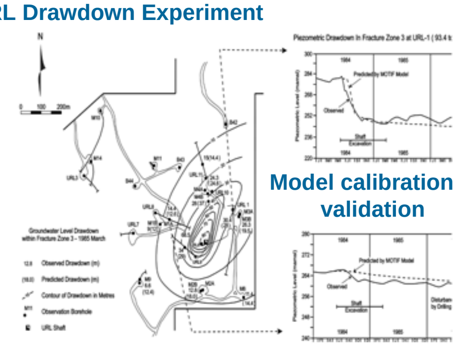
## Processes That Can be Modelled

- Stress - strain
- Rock fracture and damage
- Thermo-mechanical coupling
- Hydraulic and hydro-mechanical coupling
- Thermo-hydraulic and thermo-hydro-mechanical coupling
- Fracture flow
- Interface flow
- Solute transport
- Unsaturated to saturated swelling clay response
- Hydration of concrete



## Examples of Modelling Processes at URL

### URL Drawdown Experiment



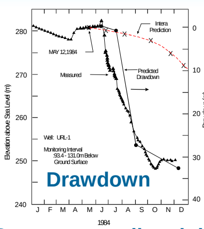
Model calibration & validation

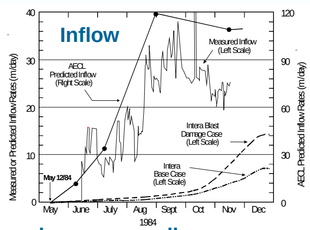
## URL Drawdown Experiment

- Pore-pressure drawdown in the moderately fractured near-surface rock was monitored at 171 locations as the URL shaft was excavated
- Finite element modelling performed to simulate both the drawdown of pore pressure caused by shaft excavation and the water inflow rate from the rock into the shaft
- The modelling performed by two different teams without prior knowledge of the results



## Comparison of Predictions & Measurements

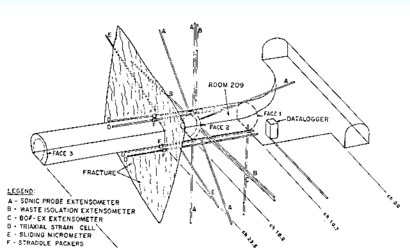



- One team predicted the drawdown very well
- Rate of inflow not well predicted (from 3 times too high to 1/3 the measured inflow)
- Modelling issues include excavation damage and stress change around the shaft that may affect fracture flow



## Excavation Through a Single Fracture



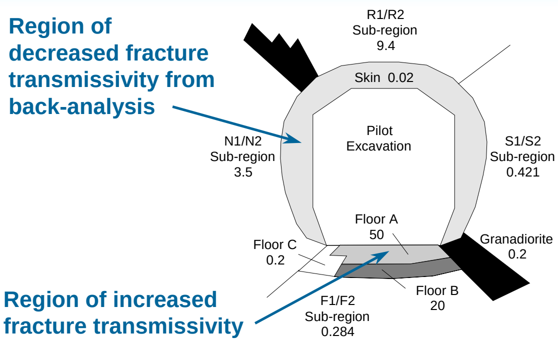

- A single fracture instrumented to measure pore pressure and stress change as excavation progressed through it
- Three modelling groups predicted the stress change, pore pressure drop and inflow into the excavations

## Excavation Response Test

- Pore-pressure change in the fracture, inflow into the excavation and stress change in the rock were poorly predicted by the modelling teams
- Stress change affected by subtle differences in the assumed *in-situ* stresses
- Pore-pressure drawdown and seepage into the tunnel affected by the assumed properties of the fracture very near the excavation
- Back-analysis provided improved understanding of the *in-situ* stress and fracture properties affected by excavation



## Back-analysis of Fracture Zone Transmissivity

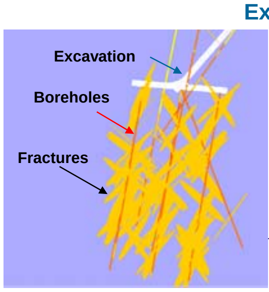



Fracture Zone Permeabilities are x $10^{-8}$ $m^2$

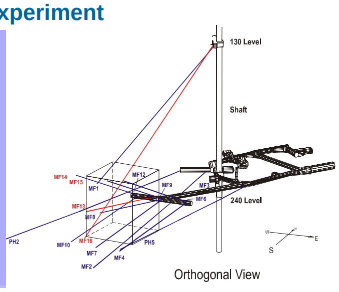


## Solute Transport Through Fractured Rock

### Solute Transport in Moderately Fractured Rock Experiment



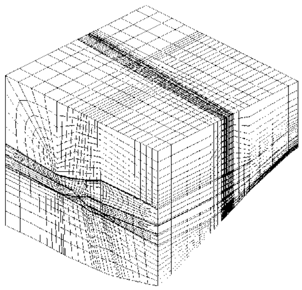

Plan View




Orthogonal View

## Flow and Transport Model Development

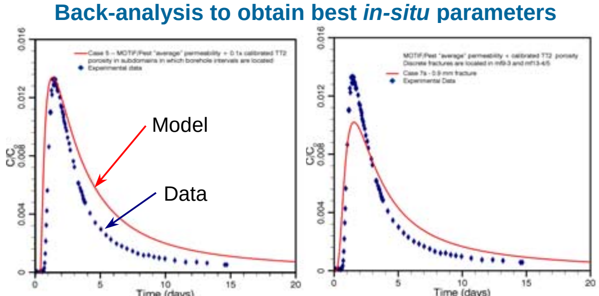
- Geometries of the various fracture domains incorporated in an Equivalent Porous Media-based finite-element model and a discrete fracture model
- Model calibrated using data from *in-situ* hydraulic characterization tests





## Computed and Measured Elution Profiles

### Back-analysis to obtain best *in-situ* parameters

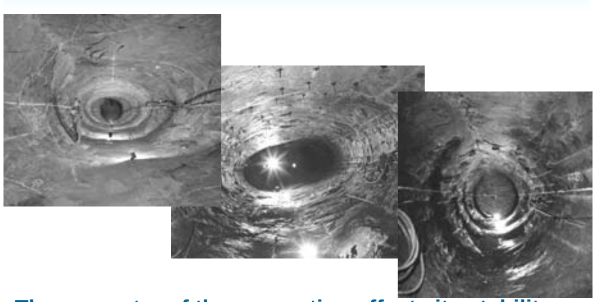



Equivalent Porous Media Model

Discrete Fracture Model

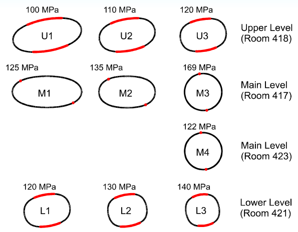


## Modelling Stability of Shaped Excavations



**The geometry of the excavation affects its stability and degree of excavation-induced fracturing within a given stress field, consistent with elastic theory**

## Excavation Stability Study




- **Ten different tunnels excavated using eight different shapes**
- **The maximum compressive stress on the excavation surface was modelled using boundary element method and closed-form solutions**



## *In-Situ* Rock Mass Strength

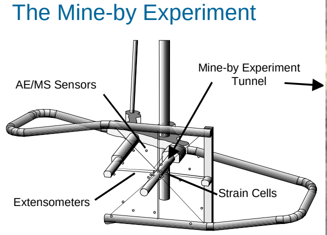
| Excavation No. | Geology | Calculated stress (MPa) | Observation | Prediction |
|---|---|---|---|---|
| U1 | Granite | 100 | No | No |
| U2 | Granite | 110 | No | No |
| U3 | Granite/ Granodiorite | 120 | No/ No | at failure/ No |
| M1 | Granite/ Granodiorite | 125 | Yes/ No | Yes/ No |
| M2 | Granite/ Granodiorite | 135 | No/ No | Yes/ No |
| M3 | Granite | 163 | Yes | Yes |
| M4 | Granite | 122 | Yes | Yes |
| L1 | Granite/ Granodiorite | 120 | No/ No | at failure/ No |
| L2 | Granodiorite | 130 | No | No |
| L3 | Granodiorite | 140 | Yes | at failure |

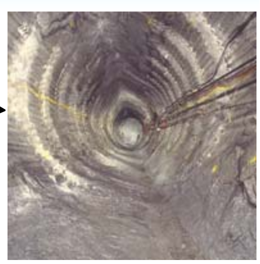
Comparing maximum calculated stress at instability (breakout) indicated the *in-situ* strength of granite (~120 MPa) and granodiorite (~140 MPa) Laboratory strengths for both are >200 MPa.



## Modelling Rock Fracturing

The Mine-by Experiment



A tunnel was mechanically excavated through an array of stress, displacement and acoustic monitoring sensors in a high-stress environment

## Mine-by Experiment

- Measured stress change and rock displacements were simulated
- The extent of cracking in the Excavation Damaged Zone (EDZ) and the size and shape of the breakout notch was simulated

### Results

- Predictive modelling of the development of rock damage was not good and had little value
- Back-analysis of the response produced a new model for *in-situ* rock failure processes that can be implemented in future work

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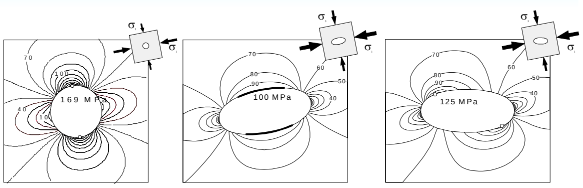
## Stress Change Caused by Excavation




- Rock mass readily modelled as an elastic solid
- Maximum compressive stress used to estimate stability
- Back-analysis of excavation-induced displacements used for accurate determination of *in-situ* stresses

*[the under-excavation stress determination method]*

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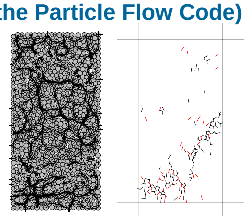
## Rock Damage

- **Prediction of rock cracking around excavations provides indication of potential for created connected hydraulic pathways in the rock along the length of tunnels**
- **Discrete element model (the Particle Flow Code) used to predict damage around various tunnels at the URL**
- **Model calibrated to results of long-term load tests performed in the laboratory**



**Force Chains** **Cracks**

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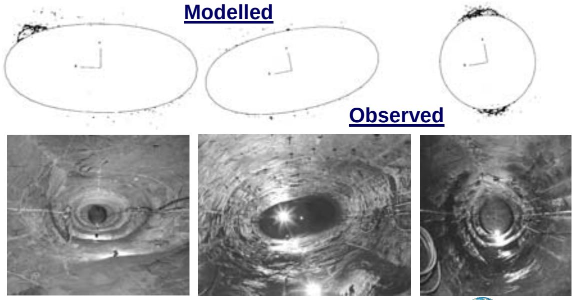
## Rock Damage

Calibrated model then used to model damage around different shaped excavations

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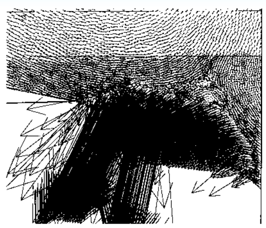
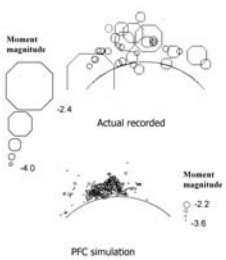
## Rock Damage

Resulting PFC model displayed many attributes of observed failure process in brittle rock






PFC model used to compute the location and magnitude of acoustic emission events around a tunnel

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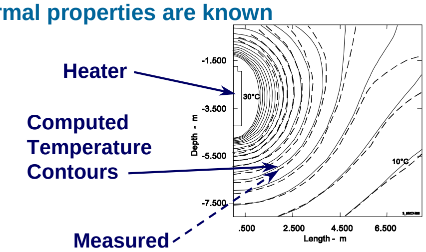
## Temperature

Experiments demonstrated that temperature change in rock and buffer can be predicted very closely if the thermal properties are known




Buffer/Container Experiment

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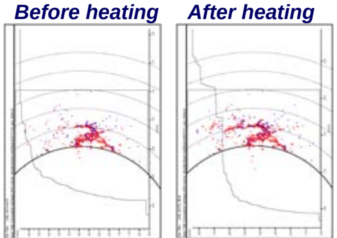
## Thermal-Mechanical Effects

- Stress increase in rock can be predicted if the *in-situ* coefficient of thermal expansion is known
- Potential for rock damage due to heating can be modelled but the validity of these models have not been tested
- Modelling rock damage around the Heated Failure Test was inconclusive

***Before heating*** ***After heating***



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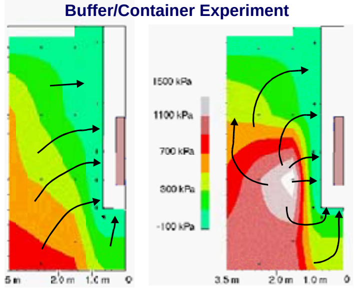
## Thermal-Hydraulic Effects

- Pore pressures are expected to increase in low permeability materials (intact rock, saturated clay, concrete) due to thermal expansion of the water
- Increase in pore pressure may cause hydraulic fracturing or may change flow direction

**Measured pore water head contours and interpreted flow paths in the Buffer/Container Experiment**




**Before Heating** **After Heating**

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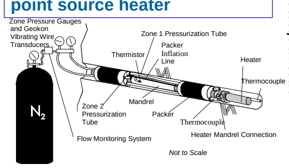
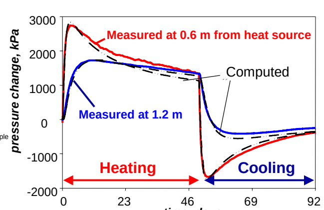
## Modelling Thermal-Hydraulic Effects

Pore pressure change in rock resulting from heating and cooling at different distances from a heat source can be modelled by using theoretical solutions of thermoporoelasticity

**Thermal-Hydraulic Experiment: measurement of pore pressure at different radii away from a point source heater**

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## Water Content in Unsaturated Clay

- Compacted swelling clay-based (bentonite) materials proposed for backfilling around containers
- Upon saturation, bentonite swells to seal construction gaps and has low permeability
- Placed unsaturated, bentonite takes on groundwater
- Material properties (strength, permeability, stiffness) and amount of swelling evolve as the material either saturates or dries from thermal effects
- Numerical models predict sealing system performance in this transient period, which could last tens to hundreds of years



## Buffer and Backfill

Buffer and backfill materials designed with different compositions of sand and bentonite. May be compacted *in situ* or in precompacted blocks. Instrumented with sensors to monitor swelling pressure and water content.

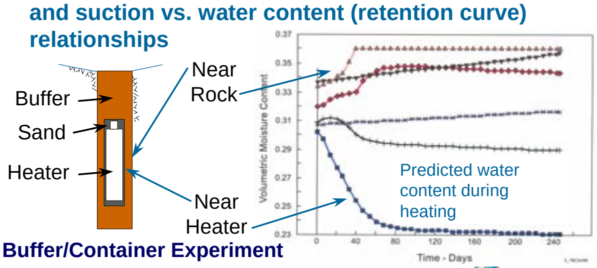
Instrumented with psychrometers

In-situ Compaction



## Water Redistribution in Unsaturated Buffer

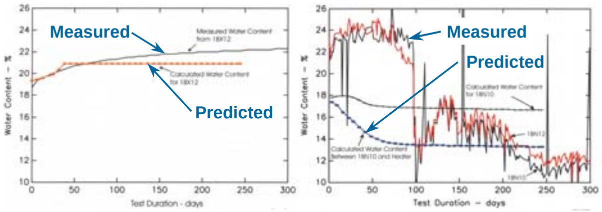
- Water-content gradient drives water movement (following Philip and DeVries formulation)
- Inputs include suction vs. hydraulic conductivity and suction vs. water content (retention curve) relationships




Buffer/Container Experiment

## Predicted vs. Measured Comparison

### Buffer/Container Experiment




**Near the rock** **Near the heater**

- Qualitatively correct trends
- Need for improved *in-situ* monitoring in the drying material

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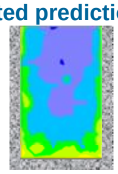
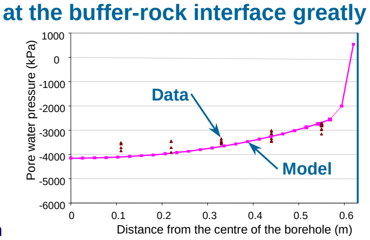
## Improving the Model

- **Ambient-temperature (no thermal gradients) experiment with water seeping from the rock**
- **Predicted pore pressure in rock and suction in buffer**
- **Assumed conditions at the buffer-rock interface greatly affected prediction**



Measured water contents
- yellow – saturated outer skin
- dark blue - initial water content

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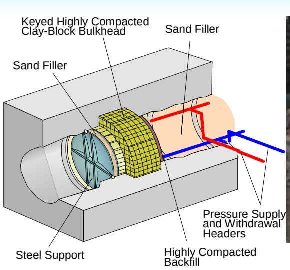
## Tunnel Sealing Experiment (TSX)




**Full-scale excavation sealed with 9000 precompacted blocks of 70% bentonite and 30% sand**

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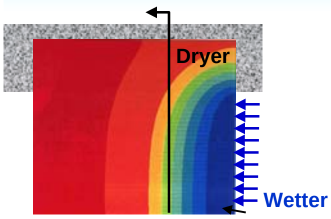
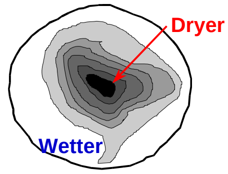
## Need for Correct Boundary Conditions



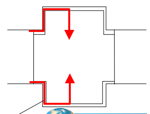

Modelled TSX Water Contents

Measurements Opposite of Predictions




Measured Cross-Section

- Actual seepage pathway along the clay-rock interface and then radially inward
- This pathway not simulated in model





## Modelling Clay-Based Materials

- **Numerical modelling tools important for predicting transient behaviour of clay backfill and buffer for optimizing engineered barrier designs**
- **Models exist that predict water movement and deformation of buffer under a variety of conditions**
- **Uncertainties remain in defining important material properties as a function of degree of saturation and in predicting many of the coupled T-H-M behaviours**
- **Chemistry and microbiology also important factors backfill models and require development**



## Summary

- **Numerical models are tools providing input to both performance assessment and repository design**
- **Models need development including validation for coupled T-H-M processes in rock, concrete and clay-based materials**
- **Laboratory tests limited for model calibration**
- **Models need testing against *in-situ* experiments**
- **For model development, back analysis of experiment data is equally important as forward prediction**

## Summary (concluded)

- Simple processes are well modelled (e.g., temperature, water flow through saturated intact rock) but coupled T-H-M process models need development
- Better instrumentation needed (e.g., moisture sensors) for quality measurements and model validation/calibration
- Special care in fully understanding boundary conditions and interfaces with other materials needed when predicting responses



## FINIS