# Used Fuel Disposition Campaign

## Summary of LBNL Modeling of Coupled Salt Coupled Processes

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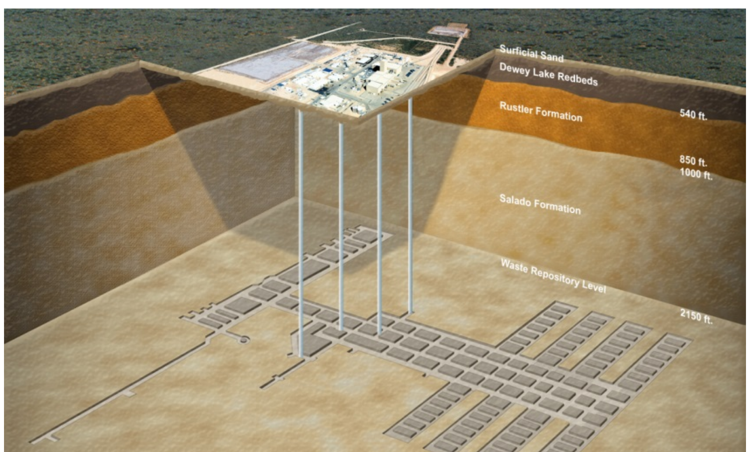
**Lawrence Berkeley National Laboratory**

**UFD WG Meeting in Las Vegas**
**Salt R&D Modeler's Meeting (I)**
**June 8, 2016**

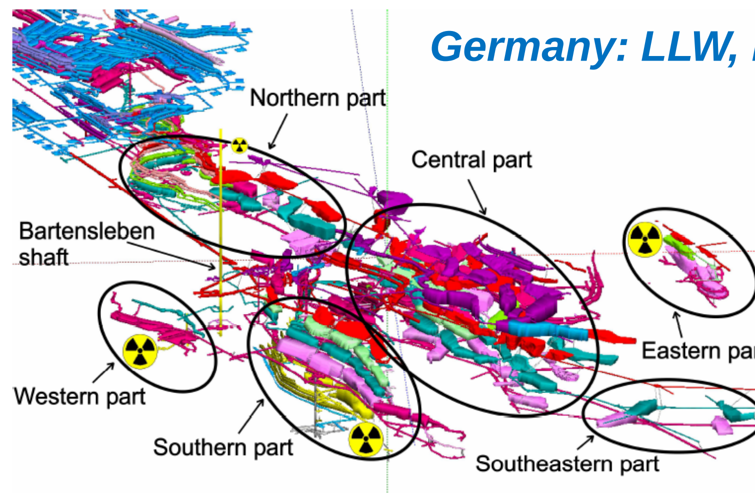
# Rock Salt is as a disposal medium

- *Advantages of rock salt*
  - *Water & gas tight*
  - *Very low porosity*
  - *Healing capability*
  - *High thermal conductivity*
  - *Stable geological areas*
  - *Easy to mine*
- *Use of rock salt as a disposal medium*




***TRU defense-related waste***

*Source: www.wipp.energy.gov*

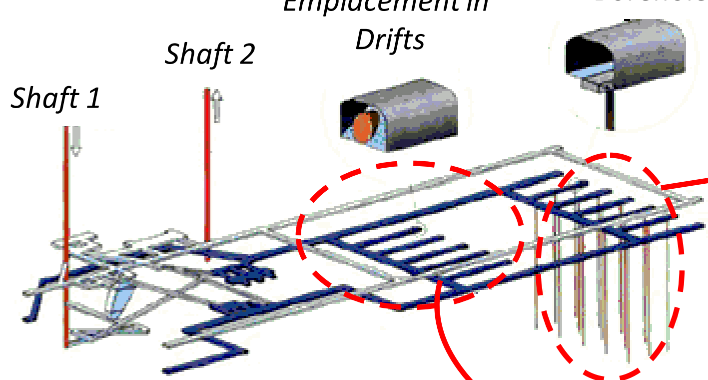



***Germany: LLW, ILW***

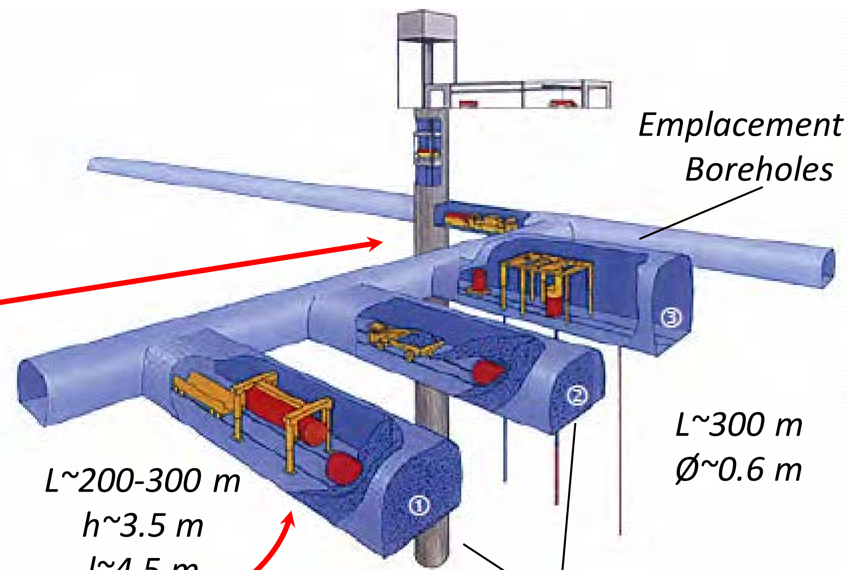
*Source: Fahland & Heusermann, 2012*

# Concept for disposal of *heat-generating* waste

*Depth ~ 600-800 m*




*Source : BAMBUS Project (1999, 2004)*




*Creep of rock salt (enhanced by temperature)* → *Closure of openings*

*Backfill compaction* → *Development of engineered barrier*

*Rock salt healing/sealing*

*Encapsulation/isolation of waste*

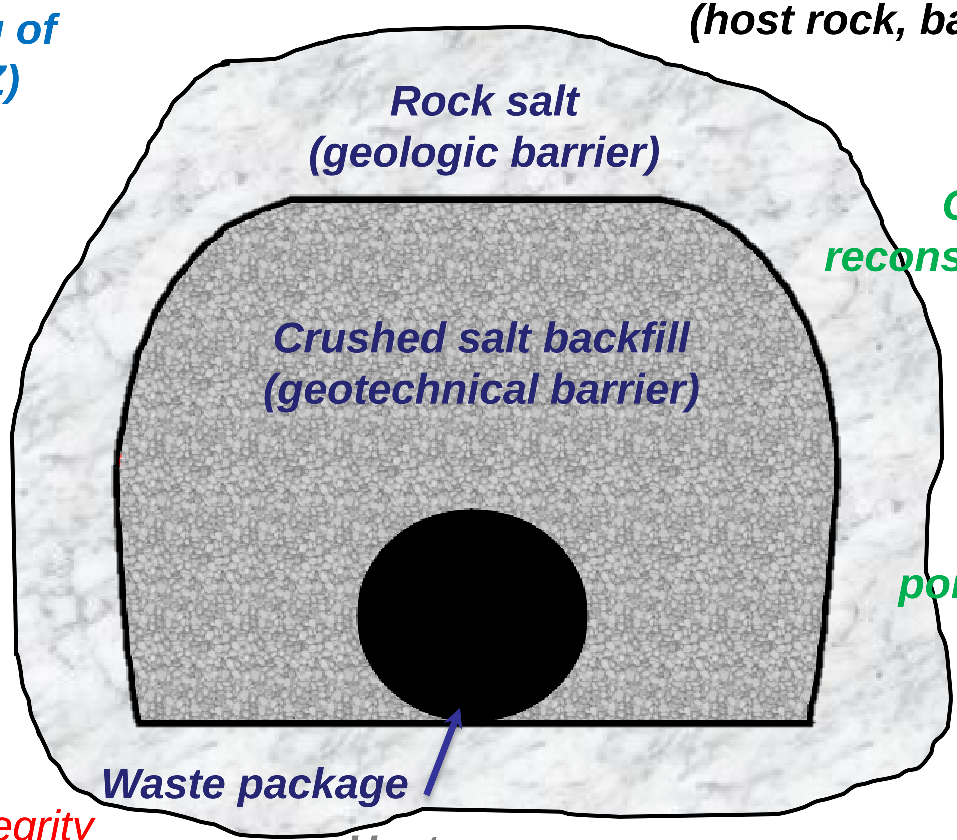
# Modeling activities at LBNL

- *Coupled THMC processes*

***Effect of brine precipitation & dissolution (host rock, backfill)***

***Damage and healing of the host rock (EDZ)***

***Fluid infiltration if $\sigma_3 + P > P_{crit}$***




***Crushed salt reconsolidation process***

***Initial crushed salt porosity ~ 30-35 %***

***Heat source, gas source (corrosion)***

*Modeling:*

- *Understanding of individual processes (infiltration, compaction, …)*
- *Predicting the long-term integrity of the barriers*

# Challenges related to salt-based materials

- *Time-dependent strain*
- *Salt is a very ductile rock:*
  - *Creep & very large deformations*
  - *Self-sealing of natural & induced defects*

*Source: TU Clausthal*

*Rock salt*


***Numerical tools need to accommodate these particularities***

***TOUGH-FLAC***

*Source:*
*BAMBUS Project*

***FLAC can handle large strains***

***TOUGH has needed updates***

***Numerical scheme adapted for creep***

*Crushed salt*

# LBNL Salt Model Coupled THM Models Timeline

- **May 2012 initiated TOUGH-FLAC salt adaptation (Milestone Sept 2012)**
  - Explored the capabilities of TOUGH-FLAC for modeling salt
  - Established collaboration with Professor Lux at Clausthal University in Germany
  - Applied TOUGH2 and FLAC3D and the Lux/Wolters for salt infiltration and creep
  - First TOUGH2 thermal-hydrologic simulation test of a generic repository tunnel in salt
- **FY13: Implementation of constitutive models and testing (Milestone Sept 2013)**
  - Implementation and testing of Lux/Wolters model into TOUGH-FLAC
  - Validation against laboratory experiments on damage induced permeability change
  - First TOUGH-FLAC simulation of a generic repository (creep over 100,000 year)
  - Developed alternative algorithms for hydromechanical coupling under large strain
- **FY14: Model improvements and testing (Milestone Sept 2014)**
  - Voronoi discretization for accurate flow simulation under (large-strain) deforming numerical grid
  - Implemented more accurate representation of damage and healing processes
  - Updated simulation of long-term THM evolution for a salt-based repository
  - Code-to-code verification of TOUGH-FLAC and FLAC-TOUGH codes
  - Developed a conceptual model for a dual-continuum approach for brine migration (involving both intercrystalline flow and intracrystalline brine inclusions)
- **FY15: Model improvements, verification and validation (Milestone Sept 2015)**
  - Initiated pore-scale (or micro-) modeling of salt inclusion migration
  - Updating our generic repository THM model and conducted updated simulations of the long-term THM behavior
  - Conducted the first full 3D (86,000 elements) TOUGH-FLAC modeling of a salt repository (heater experiment); the TSDE test in Asse Mine.
  - Extended TOUGH-FLAC for considering salt precipitation and dissolution, THMC.

# FY16 Accomplishments and Plan

Further development, verification, validation, application and publications:

- **A peer-reviewed journal paper just published**
  - Blanco-Martín et al. (2016) “Thermal–hydraulic–mechanical modeling of a large-scale heater test to investigate rock salt and crushed salt behavior under repository conditions for heat-generating nuclear waste” *Computers and Geotechnics*.
- **Completed code validation against the Asse Mine TSDE experiment**
  - The first full 3D (86,000 elements) TOUGH-FLAC modeling of salt repository (heater experiment)
  - Also TOUGH-FLAC vs FLAC-TOUGH verification with Clausthal group
- **Code validation considering salt precipitation (THMC)**
  - Validation against laboratory experiments and code-to-code verification with Code-Bright
- **Code validation for temperature evolution in crushed salt**
  - Validation against LANL laboratory heating experiment
- **Code validation for THM-induced brine release and flow in salt host rock**
  - Validation against WIPP room A brine release experiment
- **Evaluate impacts of halite solubility constraints on long-term behavior**
- **Complete pore scale modeling of brine inclusions with interpretation of Caporuscio’s experiment**
- **Implementation of dual-continuum approach for brine migration in TOUGH-FLAC (including effects of fluid inclusion migration towards heat)**

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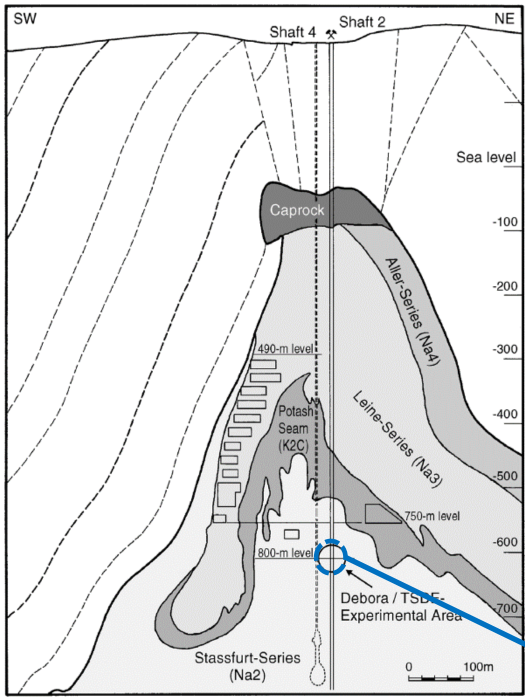
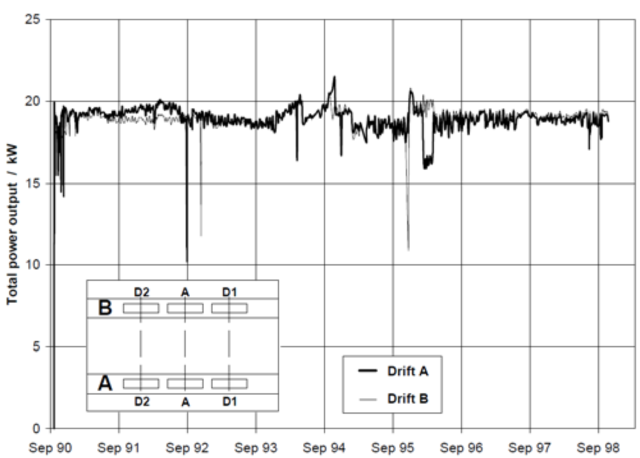
# Thermal Simulation for Drift Emplacement (TSDE) test

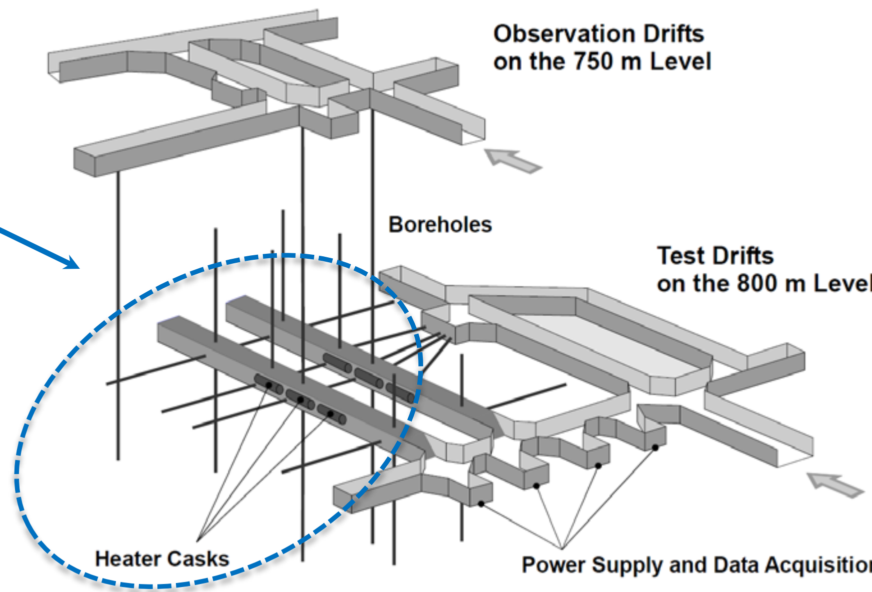



- *Asse salt mine (Germany)*
- *Conducted from 09/1990 to 02/1999*
- *About 800 m depth (salt dome)*
- *Two parallel drifts*
- *Three electric heaters/drift*
- *Constant heat load (6.4 kW/heater)*
- *Crushed salt backfill (< 45 mm)*

***Main Objectives***

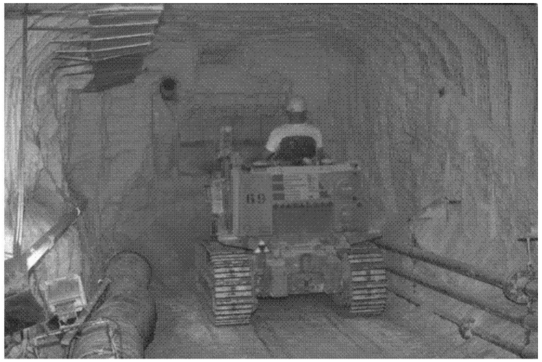
- *Feasibility of in-drift emplacement concept*
- *Study host rock & backfill under repository conditions*
- *Develop constitutive models and codes*
- *Post-heating evaluation (dismantling)*



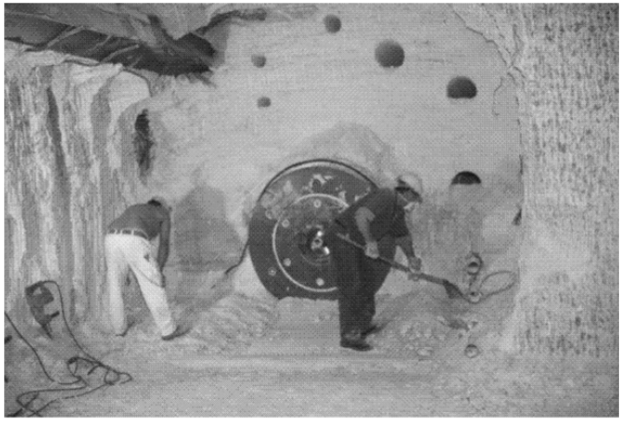



# Thermal Simulation for Drift Emplacement (TSDE) test

- **Extensive measurement campaign:**
  - Temperature
  - Drift closure & rock deformation
  - Stresses
  - Backfill setting & compaction
  - Gas generation & transport
  - Dismantling: permeability, EDZ, …




*Source : Pudewills & Droste (2004)*



*Source : BAMBUS Project (1999, 2004)*

# 3D Modeling of the *TSDE* Test

- *Nonisothermal, 2 phase flow of water & air*
- *Mechanical constitutive models:*
  - *Natural salt: Lux/Wolters model*

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}^{e}_{ij} + \dot{\varepsilon}^{vp}_{ij} + \dot{\varepsilon}^{d}_{ij} + \dot{\varepsilon}^{h}_{ij}$$

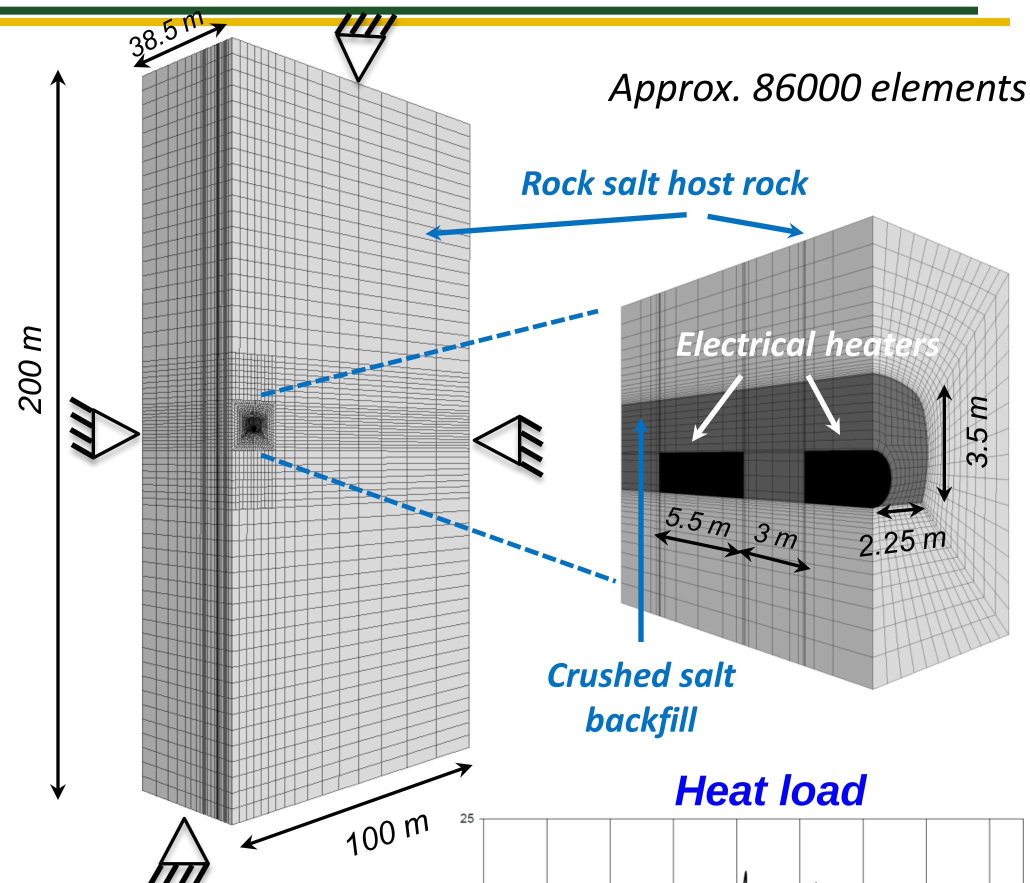
  - *Crushed salt: modified cwipp model*

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}^{e}_{ij} + \dot{\varepsilon}^{vc}_{ij} + \dot{\varepsilon}^{vs}_{ij}$$

- *Modeling sequence:*
  1. *Primary state*
  2. *Excavation (instantaneous)*
  3. *Open Drift phase (1.4 years)*
  4. *Test (8 years)*

| | Rock salt | Crushed salt |
|---|---|---|
| $S_{l,0}$ | 0.5 | 0.02 |
| $\phi_0$ | 0.2 % | 35 % |
| $k_0$ [m$^2$] | 0 | $3 \cdot 10^{-13}$ |
| $\lambda_0$ [W/m/K] | 5 | 0.9 |
| $K_0$ [MPa] | 16,650 | 150 |
| $G_0$ [MPa] | 7,690 | 70 |

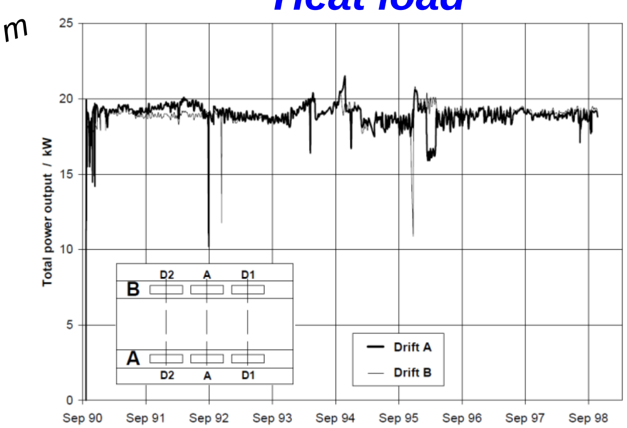
*Approx. 86000 elements*



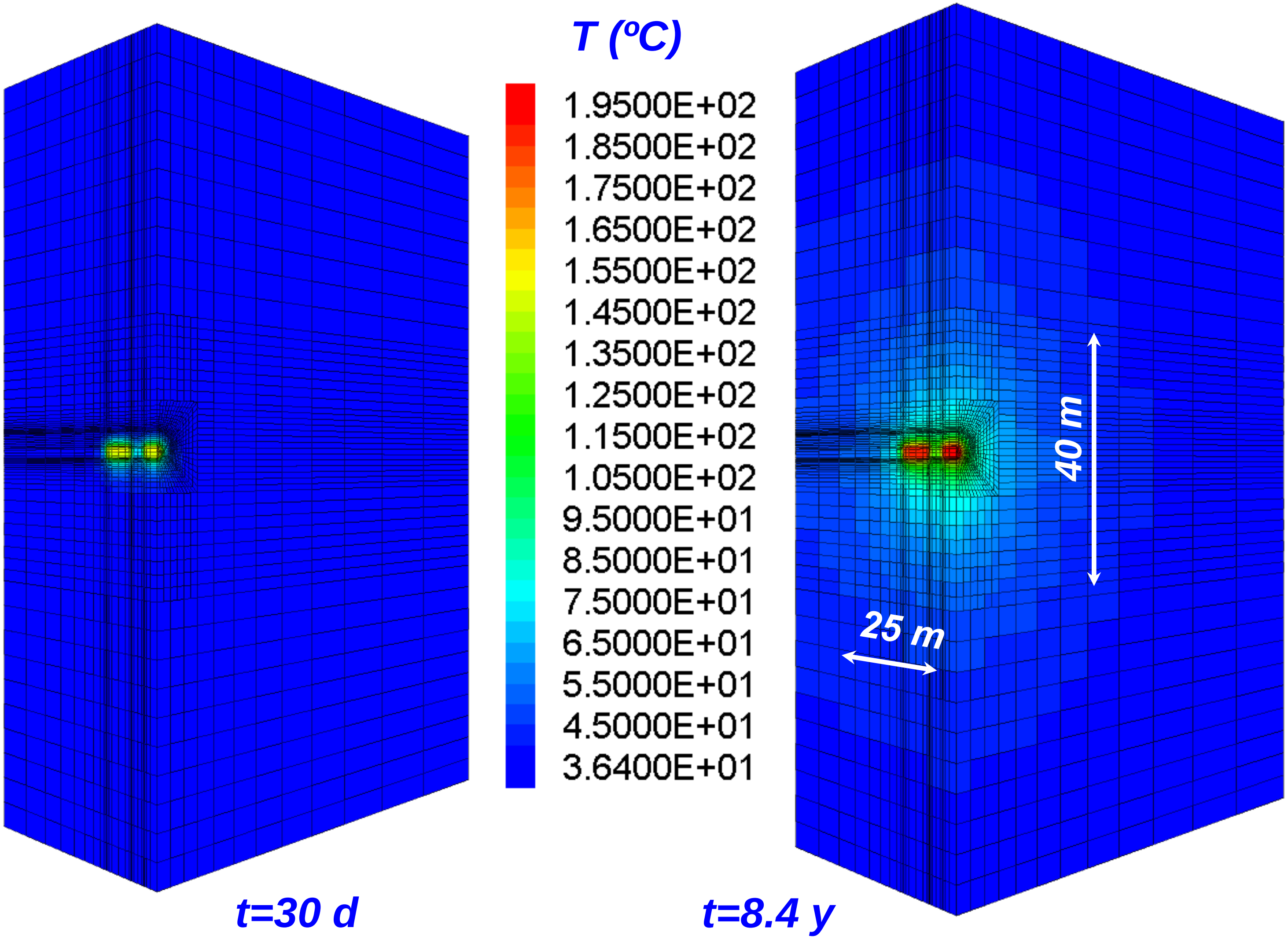

*$T_0$=36.4 ºC*

*Initial stress field: $\sigma_x=\sigma_y=\sigma_z\approx 12$ MPa*

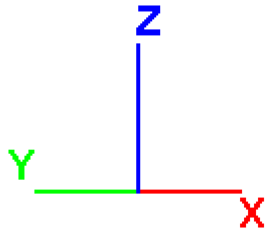
**Heat load**



# Temperature Evolution




*Progressive heat propagation through the host rock*



# Modeling of the *TSDE* test for code validation and verification

## Use of two simulators for THM modeling

*TOUGH-FLAC (Berkeley Lab)*

*FLAC-TOUGH (TU Clausthal)*

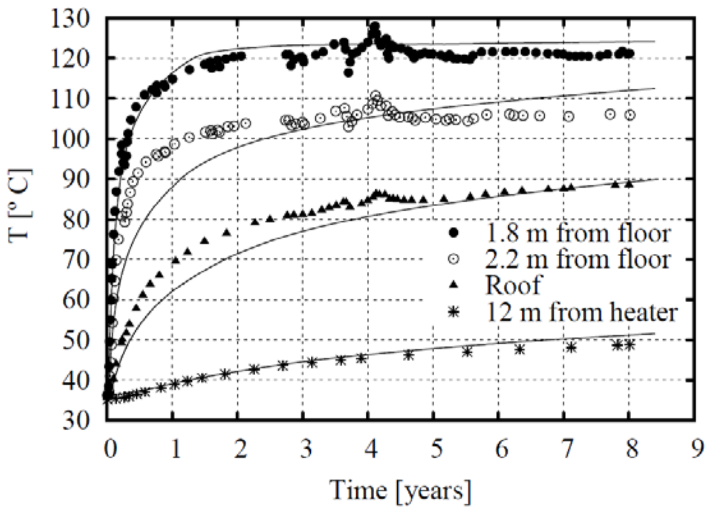
***Similarities***

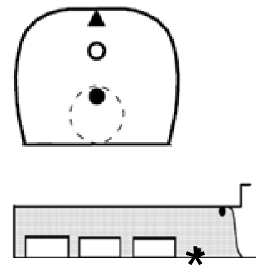
- *Based on same software*
  - *TOUGH2 (fluid + thermal flow)*
  - *$FLAC^{3D}$ (geomechanics)*
- *Sequentially coupled flow-geomechanics simulators*
- *Material-specific constitutive relationships available*
- *Can deal with large strains & creep processes*

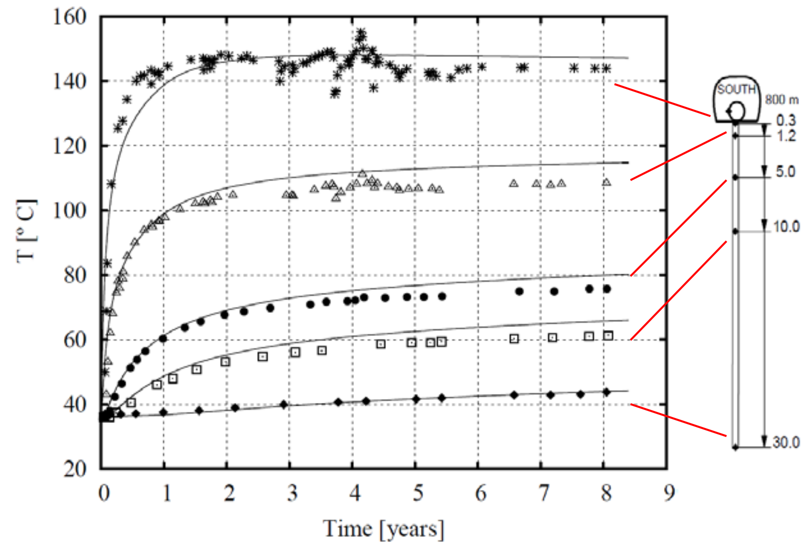
***Main difference*** → *Use of different numerical schemes*

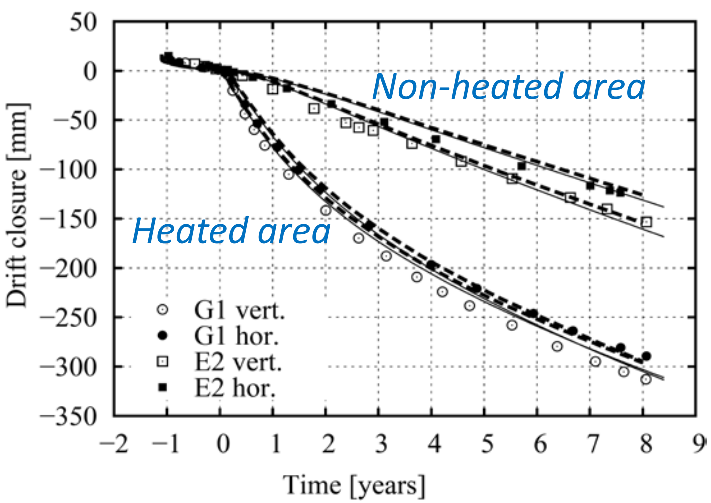
- *Fixed-stress split*
- *Undrained split*

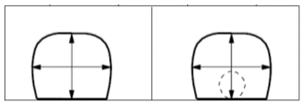
# Thermal Simulation for Drift Emplacement (TSDE) test: Modeling and Field Data

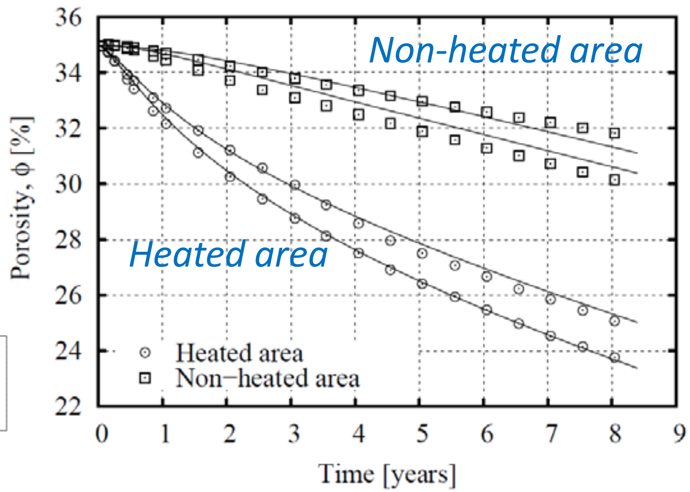




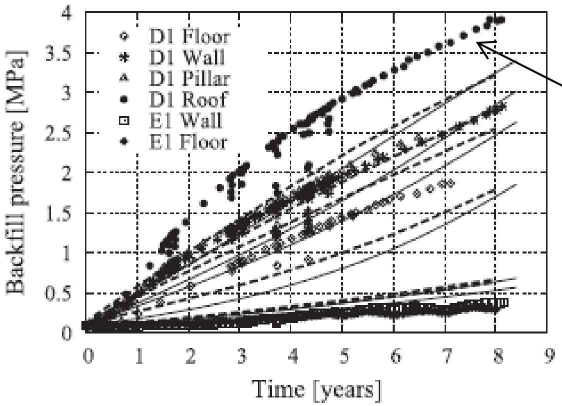



Good agreement between model and field data related to temperature and closure

# Some Findings Related to Closure and Reconsolidation of Backfill

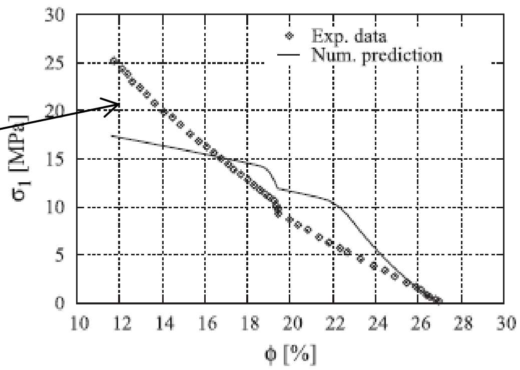
## 1) The need for improved constitutive model on compaction of crushed salt under elevated temperatures

*Backfill Stress at TSDE*




*Some deviation between model and data*

*Odometer Test*



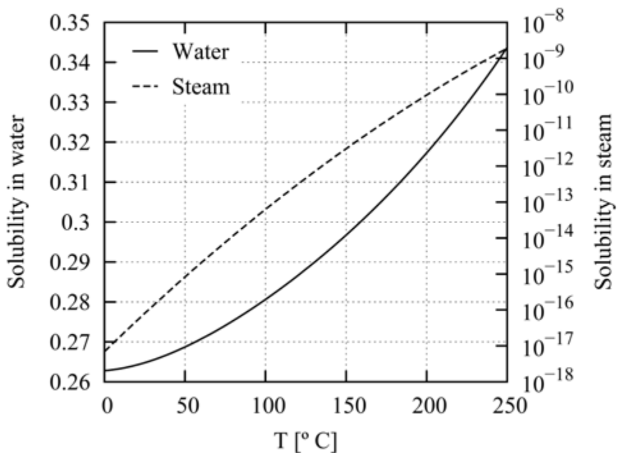

## 2) Model input parameters to capture creep processes under very small deviatoric stress had to be adjusted to match in situ measurements of drift closure.

Previous laboratory derived parameters did not capture this range and would therefore not accurately predict log-term in situ behavior.

**Still uncertainties as to how long it will take to close the drift and reconsolidate the backfill to solid intact salt**

# Added Capability of Halite dissolution/precipitation considering solubility constraints

*Halite is very soluble in water → brine*
*Solubility increases with temperature*
*Dissolution/precipitation of salt*




*Source: Driesner and Heinrich (2007); Palliser and McKibbin (1998)*

*Effective porosity (for mobile fluids)*

$$\phi_{eff} = \phi(1 - S_s)$$

*Permeability alterations, e.g.*

$$k = \exp(\beta \Delta \phi)$$

***New addition***

*Flow sub-problem:*

- *EWASG Equation-of-State (Water, Salt, Gas)*
- *Three components:*
  - *Air, water, halite*
- *Three phases:*
  - *Aqueous, gas, solid*
- *Thermo-physical properties of brine and halite (new correlations used)*
- *Phase transitions account for halite*
- *The solid phase (halite) is not mobile*

*Geomechanics sub-problem:*

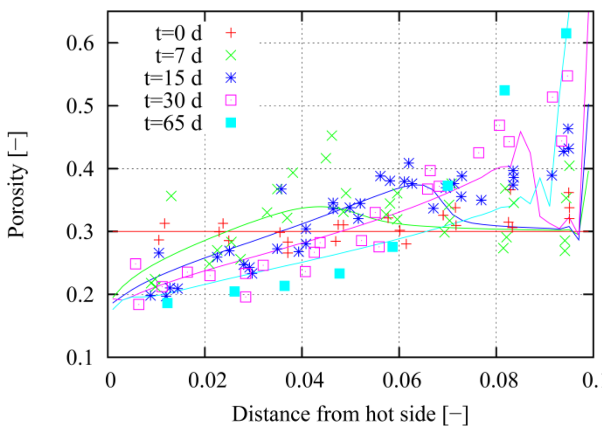
- *Backfill compaction: only the effective porosity is subject to compaction*

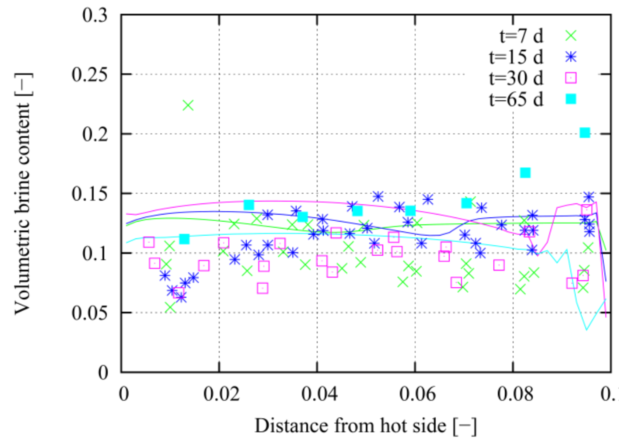
# NaCl solubility constraints: Validation against Experiments

1. *Crushed salt under temperature gradient (Olivella et al., 2011)*
   - *Lab-scale experiments, closed system, deformation blocked*
   - $\phi_0$*=30%;* $S_{l,0}$*=40%*

$T_{max}$=85 ºC

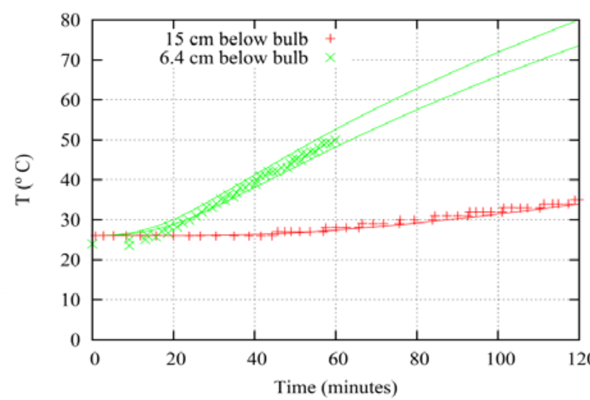

$T_{min}$=5 ºC

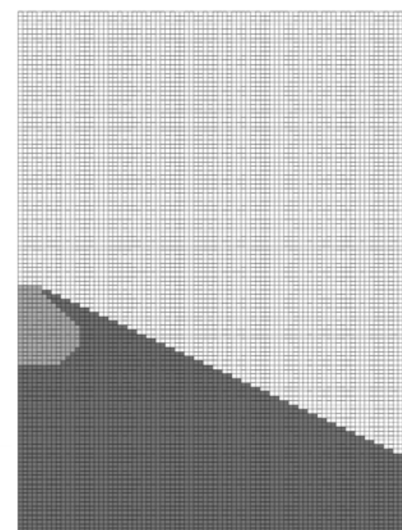



2. *Crushed salt under temperature gradient (Stauffer et al., 2013)*
   - *Lab-scale experiments, open system, pile of crushed salt*
   - *125 W for 2 h,* $\phi_0$*=37.5%;* $S_{l,0}$*=1%*

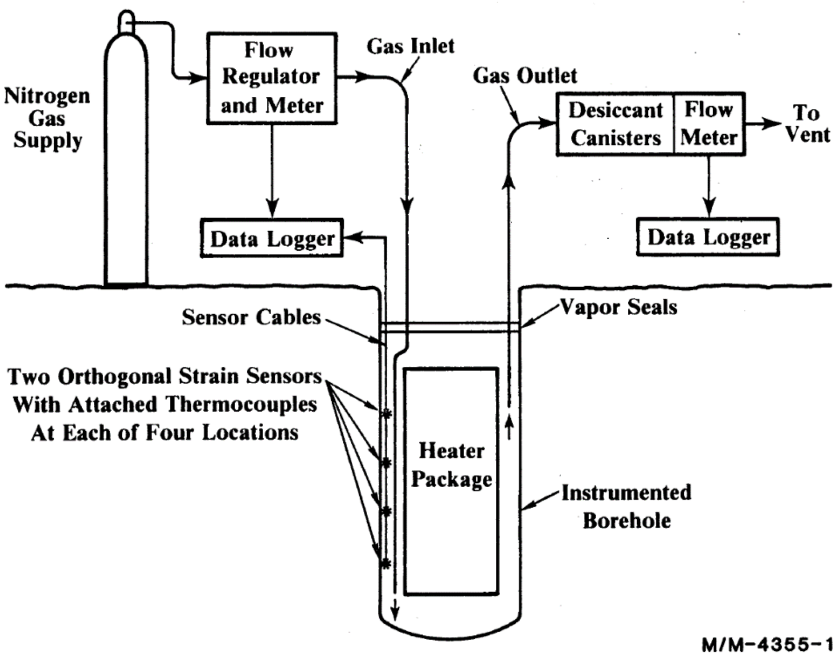
*h=31 cm*



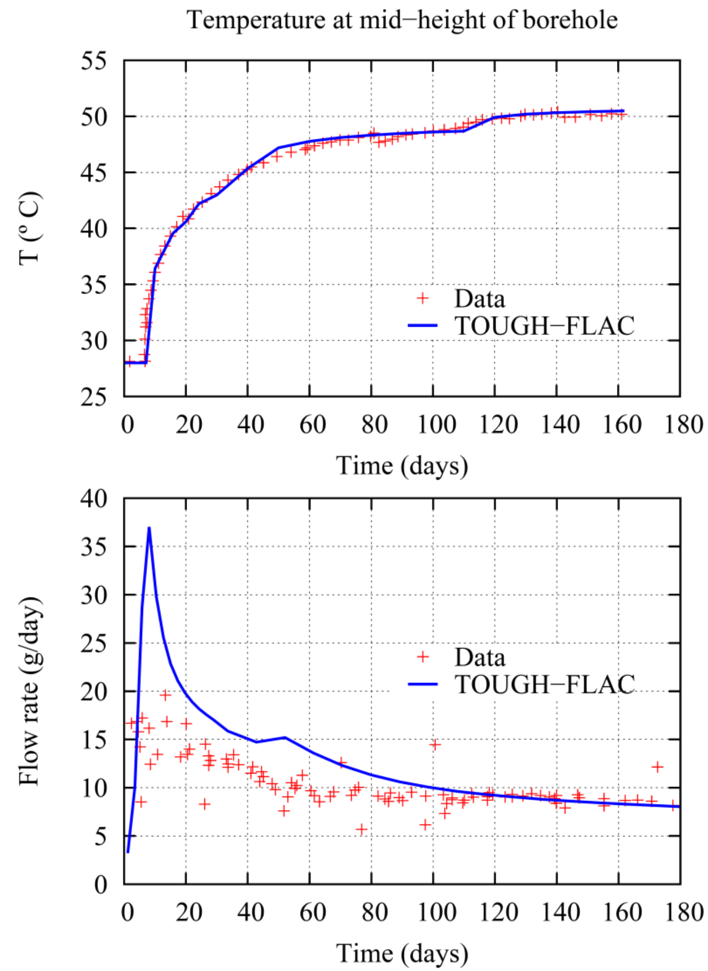



# Model validation against brine release and inflow experiment

3. *Field experiment at WIPP, room A (Nowak and McTigue, 1986)*
   - *Brine inflow under ambient conditions and under heat loading (470 W)*
   - *Measurements: temperature, cumulative water, hoop and vertical strains*




*Source: Nowak and McTigue (1986)*

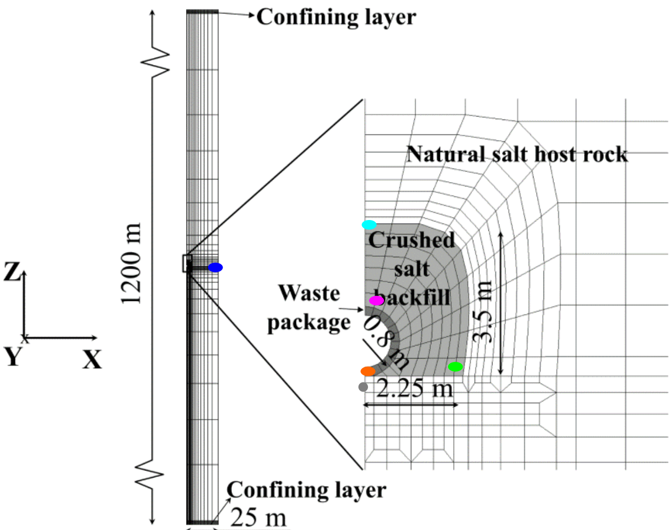



*THM simulation*

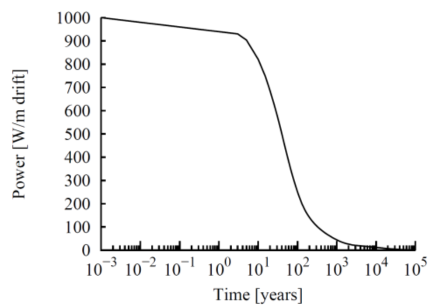
# Used Fuel Disposition

# Long-term predictions of a Generic Salt Repository

## *2D model*

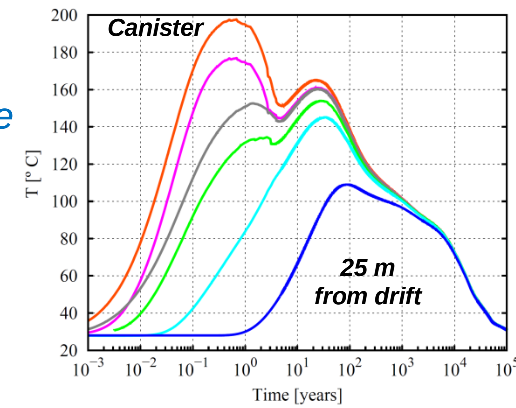



## *Heat load*

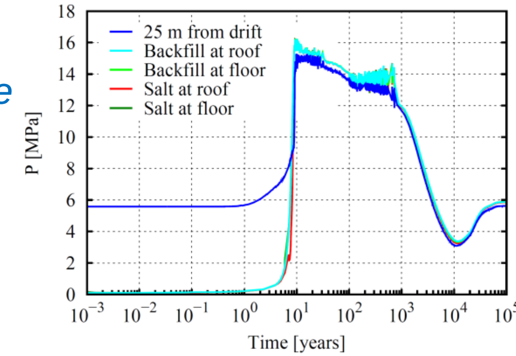



*Source: Carter et al., 2011*

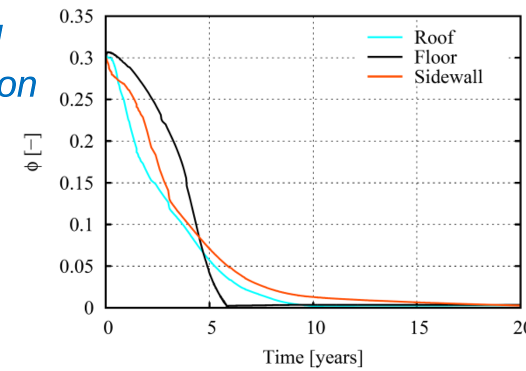
## *Temperature*



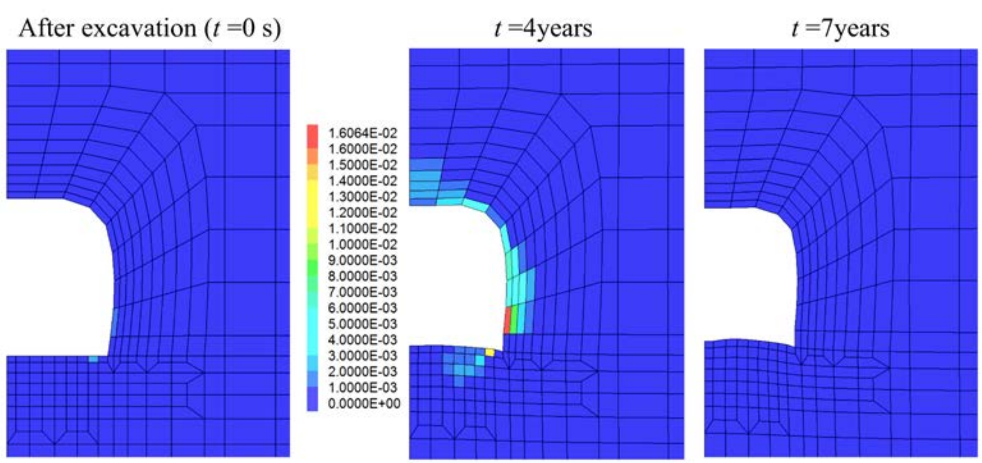

## *Pore pressure*




## *Backfill compaction*

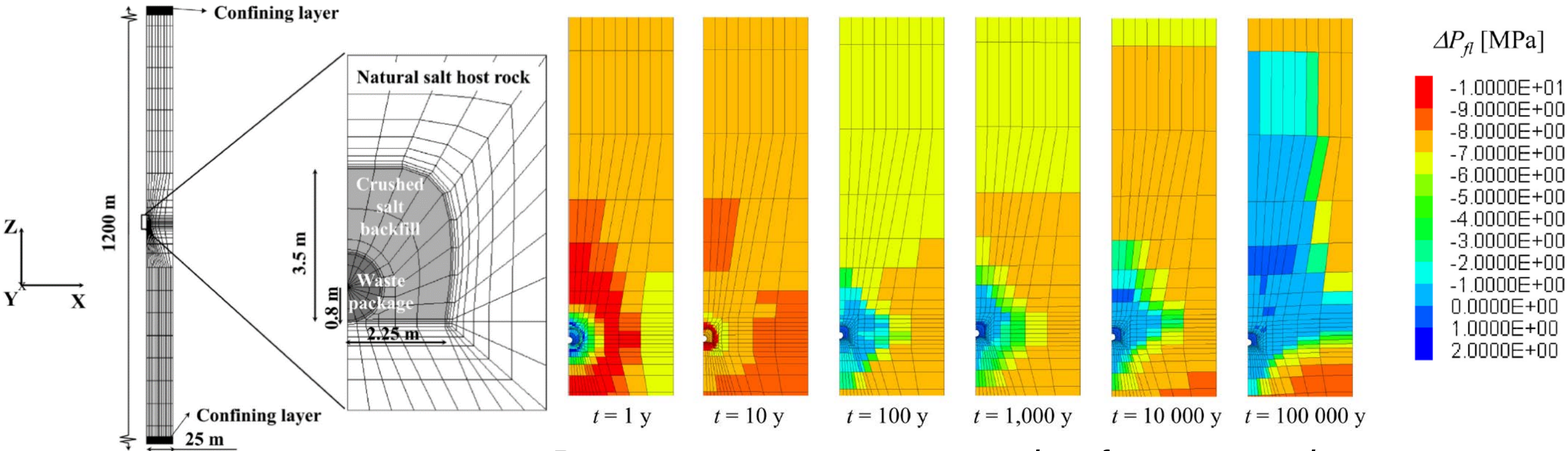



## *Dilatancy/healing*

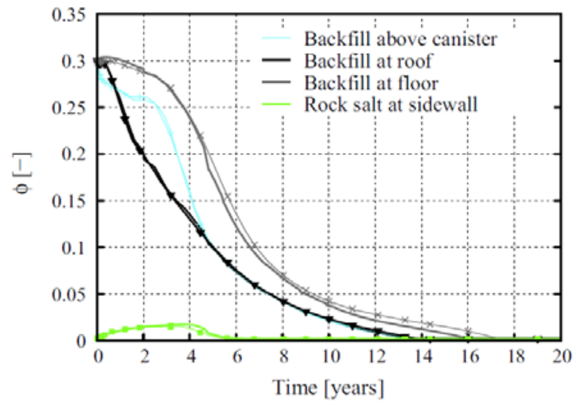


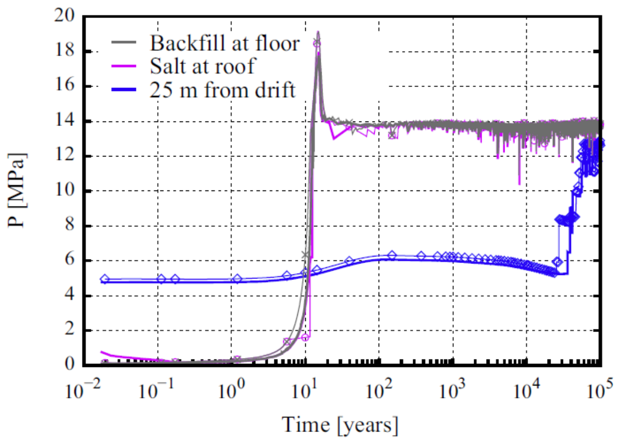
# Salt Coupled THM Processes – TOUGH-FLAC

***Example THM induced flow in the near field:***




*Pressure permeates as a results of gas generation*

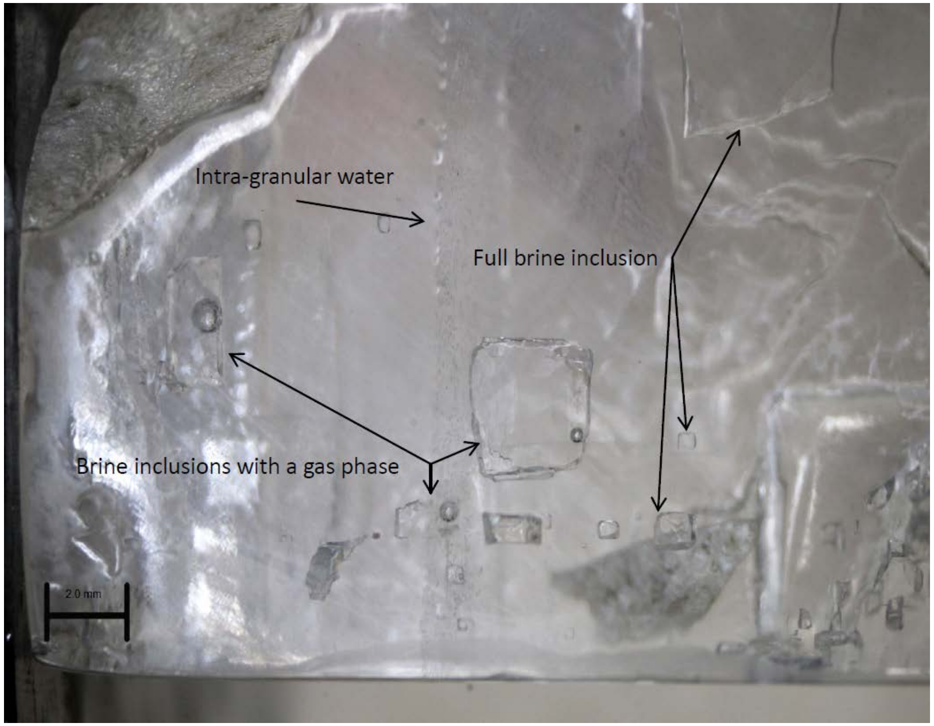


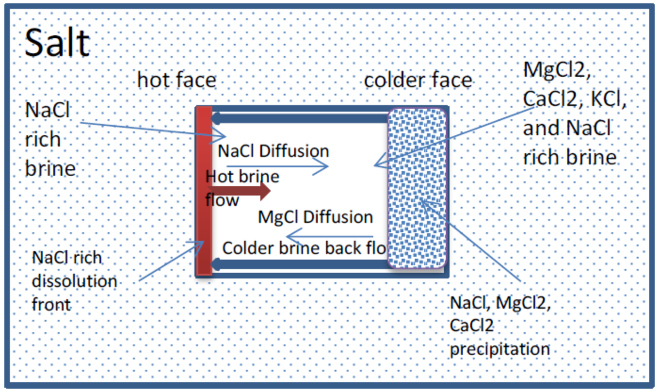
# Pore-Scale Simulation of Brine Inclusion Migration

**Simulations by S. Molins (EESA) and D. Trebotich (CRD)
Lawrence Berkeley National Laboratory**

**Caporuscio et al, 2013**, Brine migration experimental studies for salt repositories, FCRD-UFD-2013-000204




- Individual brine inclusions were mobilized when subjected to thermal gradients.
- Brine migrated toward the heat source
- Brine migration occurred through a network of micron size channels created along the migration path.



# The pore scale approach

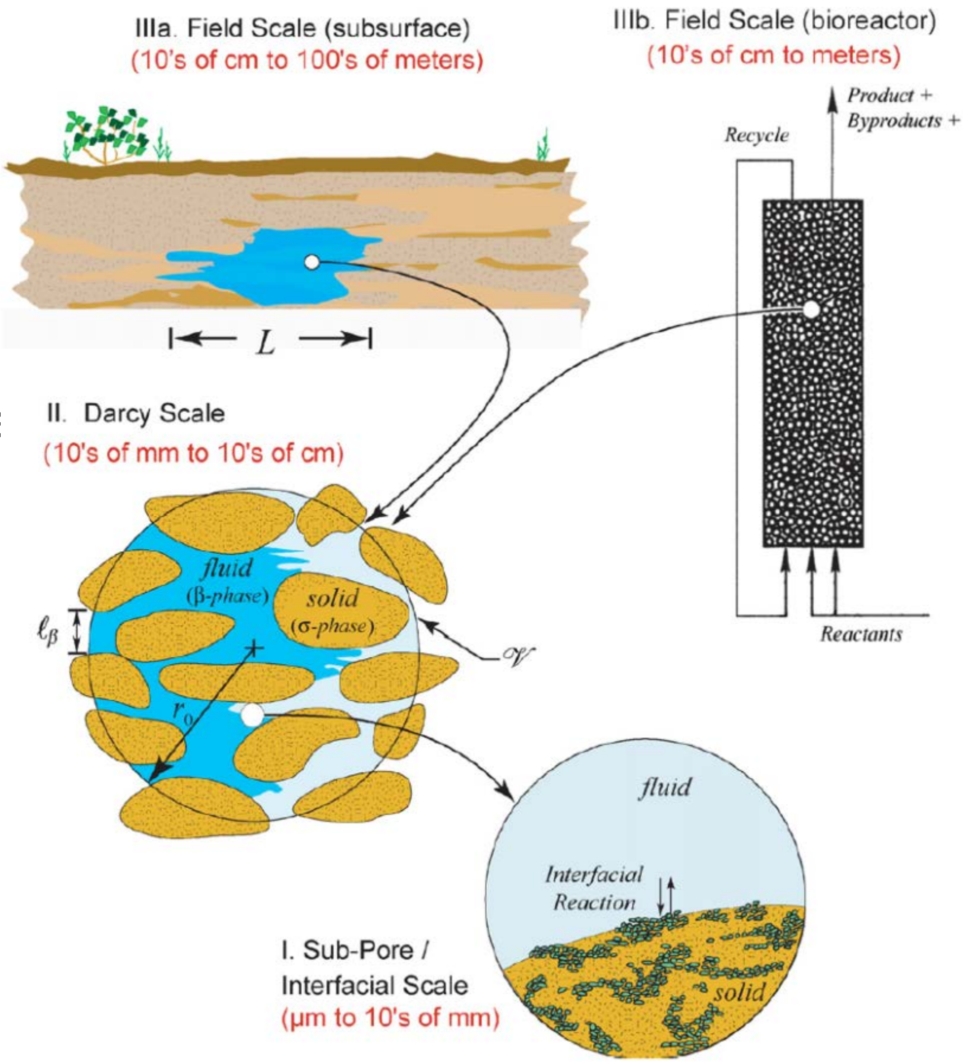
- **Darcy (continuum) scale**
  - Porous medium continuum
  - Well-mixed assumption in each cell
- **Pore scale**
  - Explicit pore space geometry
  - Different phases are distinguishable
  - Interfaces considered in models
  - Incompressible Navier-Stokes flow

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right)=-\nabla p+\mu\nabla^2\mathbf{u}$$

$$\nabla\cdot\mathbf{u}=0$$

  - Reactive transport

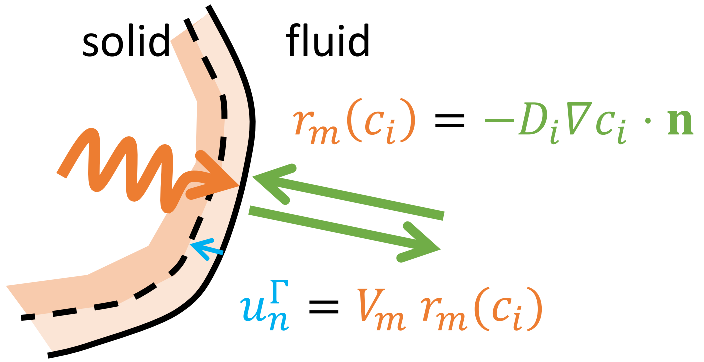
$$\frac{\partial \rho c_i}{\partial t}+\nabla\cdot\rho\mathbf{u}c_i=\nabla\cdot\rho D_i\nabla c_i$$



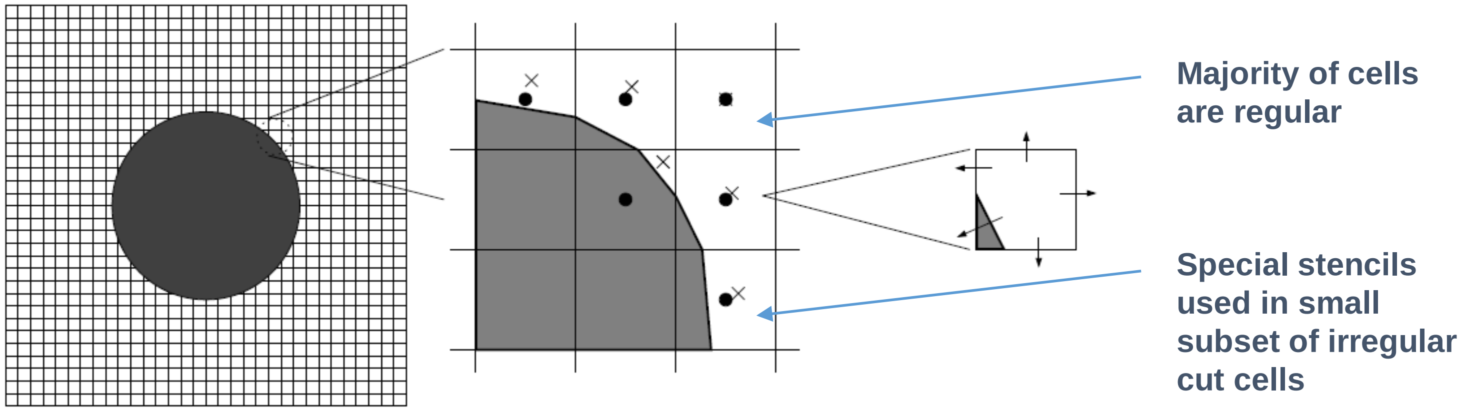

*Wood et al 2007 Adv Water Resour*

# The pore scale approach

- Surface reactions
  - Rates are calculated at the fluid-solid reactions
  - Rates depend on pore scale transport processes
  - Fluid-solid boundaries evolve as a result of dissolution-precipitation

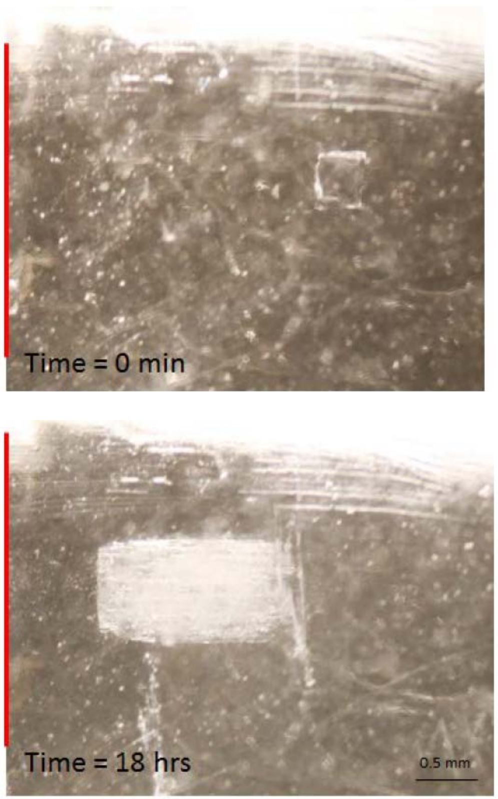



- Embedded Boundary Method
  - Finite volume method where irregular boundaries are represented intersecting pore geometry with Cartesian grid

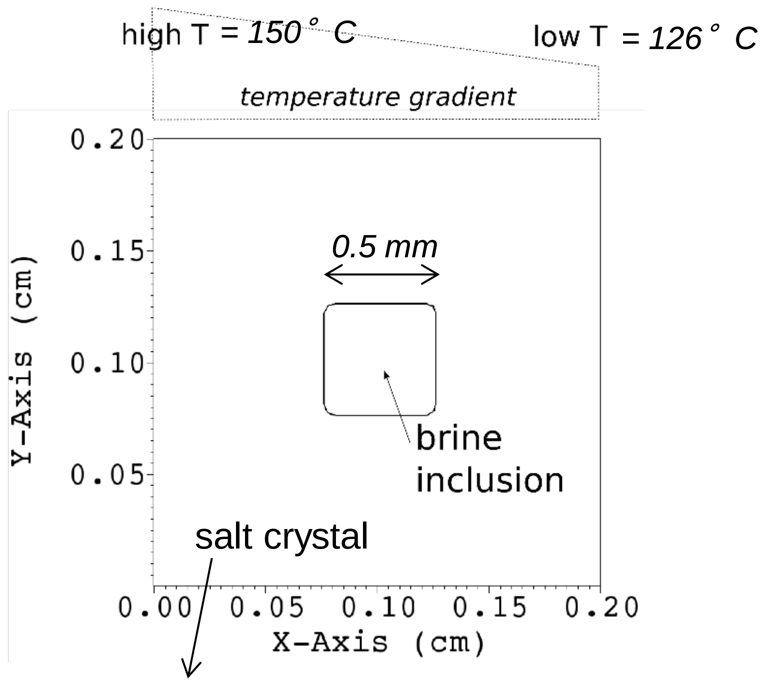



Molins et al 2012 Water Resour Res
Molins et al 2014 Environ Sci &Technol
Trebotich and Graves, CAMCoS, 2015

# Brine inclusion pore-scale model




Caporuscio et al, 2013
FCRD-UFD-2013-000204

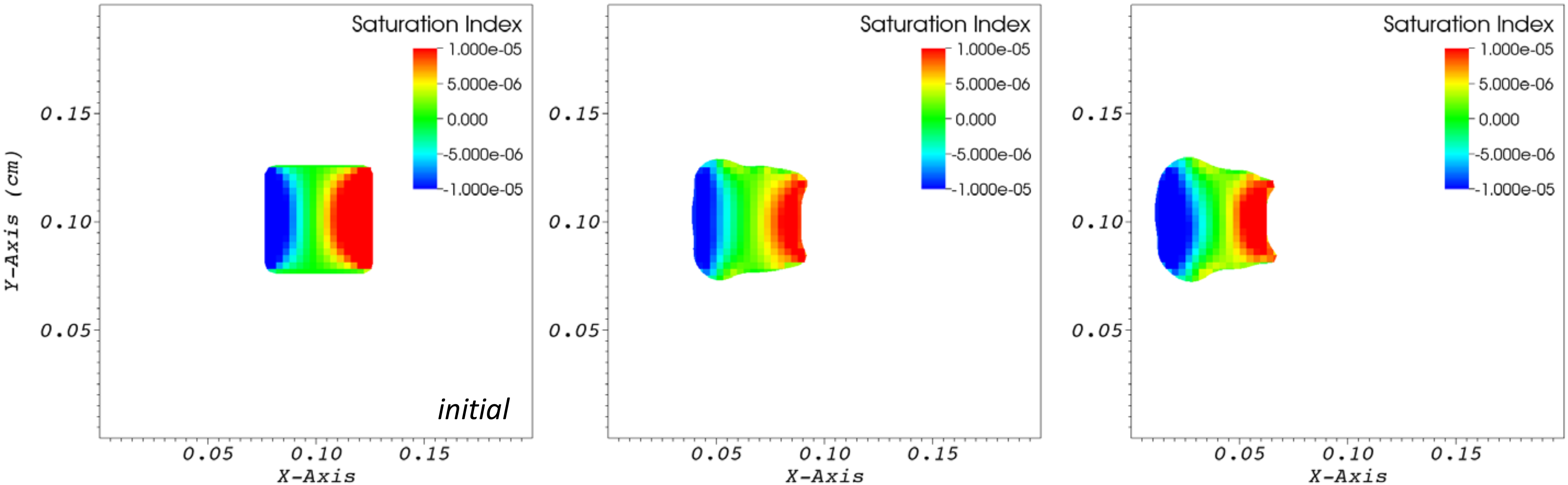



Salt crystal represented by halite, both for dissolution and precipitation

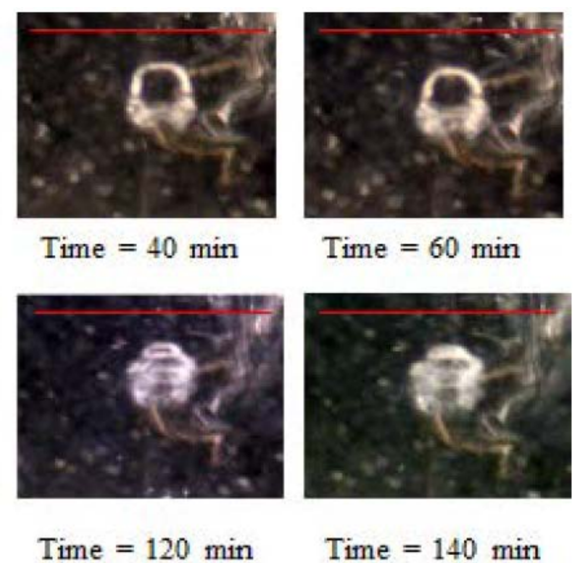
$$NaCl(s) \leftrightarrow Na^+ + Cl^-$$

$$r = k \exp\left[-\frac{E_a}{RT}\right]\left(1 - \frac{[Na^+][Cl^-]}{K_s(T)}\right)$$

# Simulated brine inclusion migration

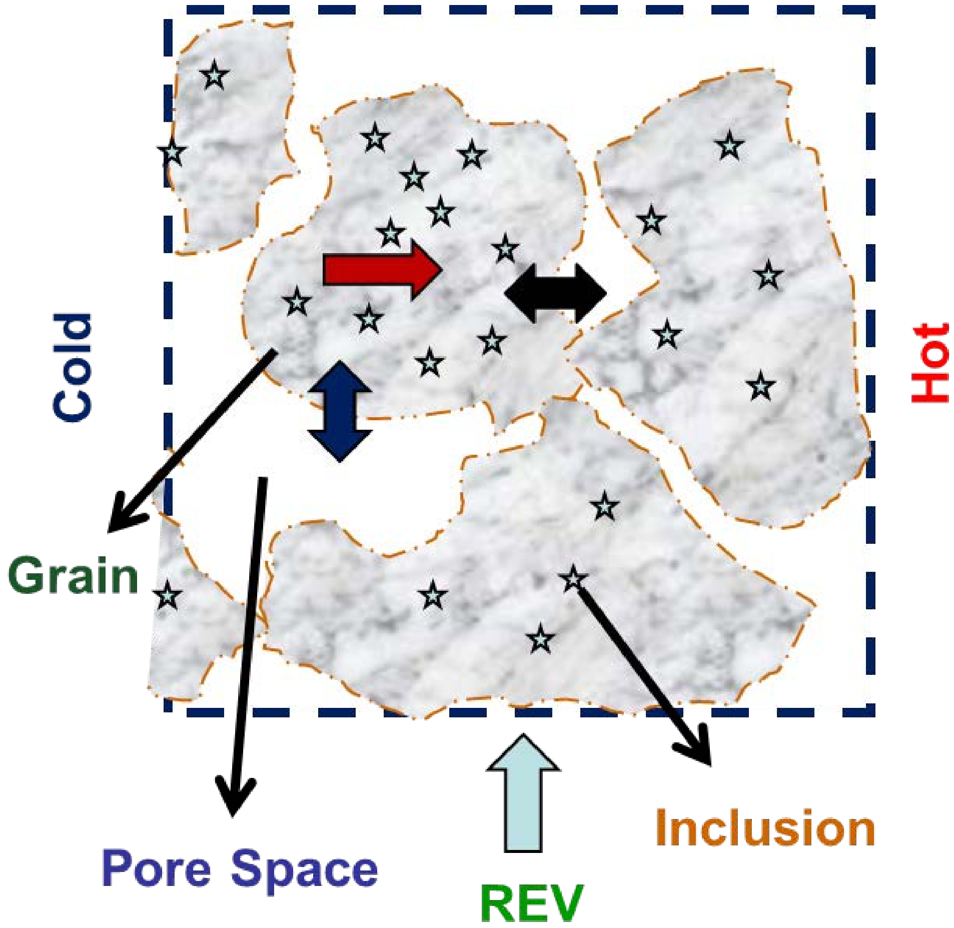



- Migration is driven by very small halite saturation gradients
- Initial shape changes are captured rather well
- Rate of migration is significantly slower (~20x) than experimental observations
- FY 2016 work focuses on understanding this discrepancy:
  - Calibration of reaction rate constant
  - Effect of temperature gradient
  - Effect of multiple minerals with different rate constants and solubilities
  - Effect of neglecting heat-driven flow




Caporuscio et al, 2013

# Dual Continuum Approach for TOUGH-FLAC to Consider Effects of Brine Inclusions




– *One continuum representing the connected intergranular pore space*

– *A second continuum representing the brine inclusions*

Dual-continuum model to be implemented and to be used for modeling brine release and brine flow around a heat source

# FEPS Associated with Coupled THM Processes Modeling

## *Associated FEPS:*

*The most closely associated FEP is 2.1.01.01 Evolution of EDZ (see below – from the UFD Roadmap spreadsheet/tables). Related FEPs are Flow Through the EBS (2.1.08.01), 2.1.08.03 (Flow through Backfill), 2.1.08.06 (Alteration and Evolution of EBS Flow Pathways), 2.1.08.09 (Influx/Seepage Into the EBS), Open Boreholes (1.1.01.01), Thermal Effects on Flow in EBS (2.1.11.10), 2.2.01.01 (Evolution of EDZ) , Flow Through Host Rock (2.2.08.01), Effects of Excavation on Flow (2.2.08.04), Mechanical Effects from Preclosure Operations (1.01.02.02), Heat Generation in EBS (2.1.11.01), Effects of Backfill on EBS Thermal Environment (2.1.11.03), Effects of Drift Collapse on EBS Thermal Environment (2.1.11.04), Effects of Influx (Seepage) on Thermal Environment (2.1.11.05), Thermal-Mechanical Effects on Backfill (2.1.11.08), Thermally-Driven Buoyant Flow / Heat Pipes in EBS (2.1.11.12), Effects of Gas on Flow Through the EBS (2.1.12.02), Gas Transport in EBS (2.1.12.03), Thermal-Mechanical Effects on Geosphere (2.2.11.06)*

| Objective | Feature | Process (Issue) | | |
|---|---|---|---|---|
| | | UFD FEP ID | UFD FEP Title | Process/Issue Description |
| Limited Release – Natural Barriers | Natural System - Geosphere | 2.2.01.01 | Evolution of EDZ | - Lateral extent, heterogeneities<br>- Physical properties<br>- Flow pathways<br>- Chemical characteristics of groundwater in EDZ<br>- Radionuclide speciation and solubility in EDZ<br>- Thermal-mechanical effects<br>- Thermal-chemical alteration |

# Importance to Safety Case/Performance Assessment

***Affect on repository performance:***

*Coupled THM processes are relatively short-lived from safety assessment perspective, but could potentially give rise to permanent changes, such as formation of a damaged zone around excavations that could provide a path for transport of radionuclides if released from a waste package.*

*As for the natural salt, it is well known that its initial tightness could be affected by processes that take place at different stages during the lifetime of a repository.*

1) *Development of an excavation damaged zone (EDZ) around the mined openings represents a potential risk because preferential flow pathways could be created.*

1) *A pore pressure-driven percolation process (fluid infiltration) can take place if the pore pressure locally exceeds the minimum compressive principal stress.*

*These perturbations, however, are generally not persistent in a plastic medium such as rock salt. Once the stress regime becomes favorable, healing takes place. Healing processes consist in the development of cohesion between former crack planes (in extension of pore space closure).*

# Link to the PA Model

- The TOUGH-FLAC with salt constitutive THM models provides a tool for calculating the evolution of the crushed salt backfill and the host rock, including the disturbed rock zone (DRZ) from just after emplacement to over 100,000 years.

- The analysis for coupling to the PA model might be conducted in a 2D cross-section of one emplacement drift or alternative a 3D model focused on the near field of an emplacement tunnel or a few emplacement tunnels in different parts of a repository and for different FEPs such as nominal case or such as for cases of extensive gas generation.

- The **input** required is the geometry, heat source, THM properties of buffer and host rock, initial THM conditions (such as in situ stress).

- The **output** to the PA model would be the changes in flow properties (e.g. permeability and porosity) in the EBS and near-field including the buffer and DRZ and also to inform PA related to local flow created by coupled THM processes.

# Uncertainty Reduction by code Validations

The coupled THM processes in salt are complex but can be analyzed using coupled numerical modeling with adequate constitutive models, verified and validated against laboratory and field tests.

- Brine infiltration laboratory experiments validating implementation of Lux/Wolter's model in TOUGH-FLAC for brine infiltration
- Triaxial compression test to validate TOUGH-FLAC with Lux/Wolter's model regarding mechanical behavior under shear stress and strain
- Modeling of Terzaghi's 1D consolidation problems with comparison to analytic solution to verify TOUGH-FLAC hydraulic and mechanical coupling algorithm
- Modeling verification against Mandel's problem solution to verify TOUGH-FLAC hydraulic and mechanical coupling algorithm
- Modeling TSDE experiment validating THM model including drift closure and crushed salt compaction at a realistic scale
- Modeling WIPP Room A THM induced brine release experiment
- Modeling salt dissolution/precipitation laboratory experiment under thermal gradient

Some remaining: Laboratory and long-term field experiment to ultimate sealing and healing under elevated temperature, brine release and migration towards heat, and sealing after high-pressure infiltration…..

# LBNL Salt Coupled Processes Modeling

## Next

- Evaluate impacts of halite solubility constraints on long-term behavior
- Complete pore scale modeling of brine inclusions with interpretation of Caporuscio's experiment
- Implementation of dual-continuum approach for brine migration in TOUGH-FLAC (including fluid inclusion migration towards heat)

## Longer Term

- Modeling support for field test design, prediction and interpretation
- Detailed brine migration studies using dual-continuum model considering thermal gradient driven migration
- Long-term THM behavior for different repository design (e.g. alcove rather than in-drift storage)
- Further code benchmarking in collaboration with Clausthal University
- Porting TOUGH-FLAC to HPC following FLAC3D's MPI version and porting to Linux (expected new few years)
- TOUGHREACT-FLAC for mechanistic THMC modeling (e.g. underlying chemo-mechanical processes of creep)?