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Sandia National Laboratories

Thermomechanical-Hydrology Modeling for HLW Disposal

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Sandia National Laboratories

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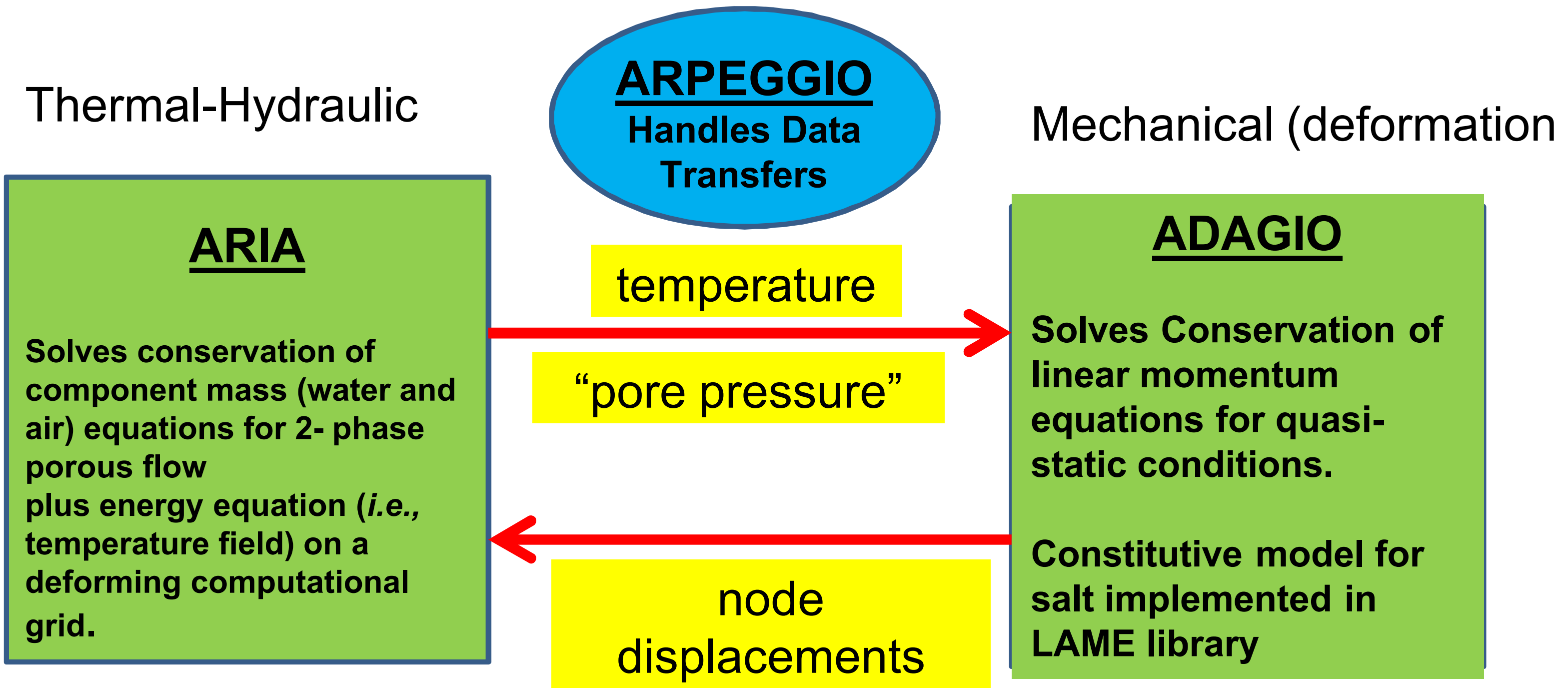
Organization of Presentation

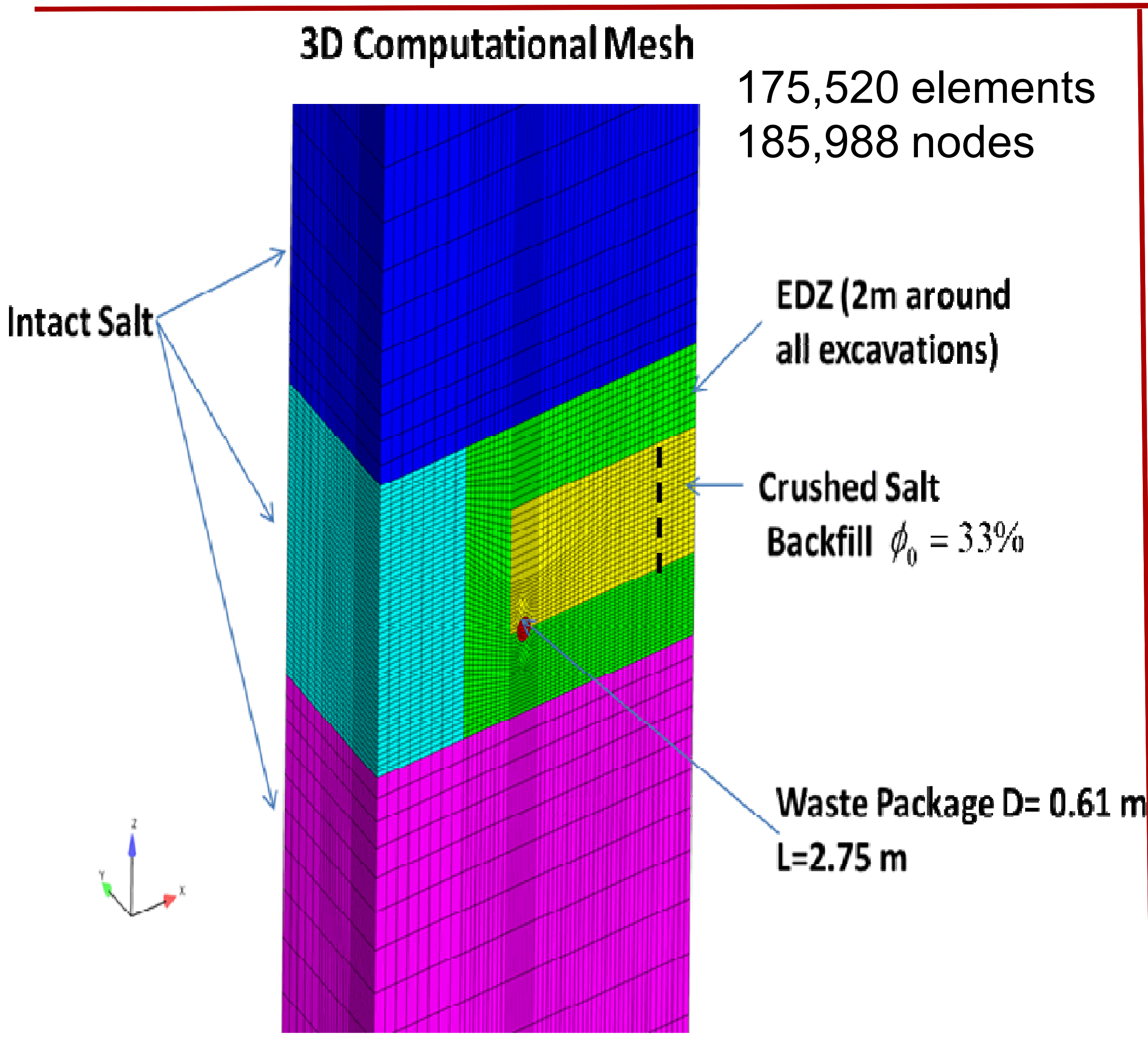
- **SIERRA Mechanics Physics Coupling Strategy**
  - Using workstation and/or massively parallel-processor computers
- **Thermal- Mechanical (TM) Modeling**
  - Constitutive model for intact and crushed salt
  - Porosity and temperature dependent thermal conductivity model
  - Results- Focus on consolidation time of the crushed salt backfill for varying values of assumed moisture content
- **Thermal-Hydraulic (TH) Modeling**
  - Thermal and 2-phase porous flow properties
  - Model moisture movement due to decay heat in the crushed salt and EDZ regions
- **Summary and Future Work**

SIERRA T-H-M Physics Solution



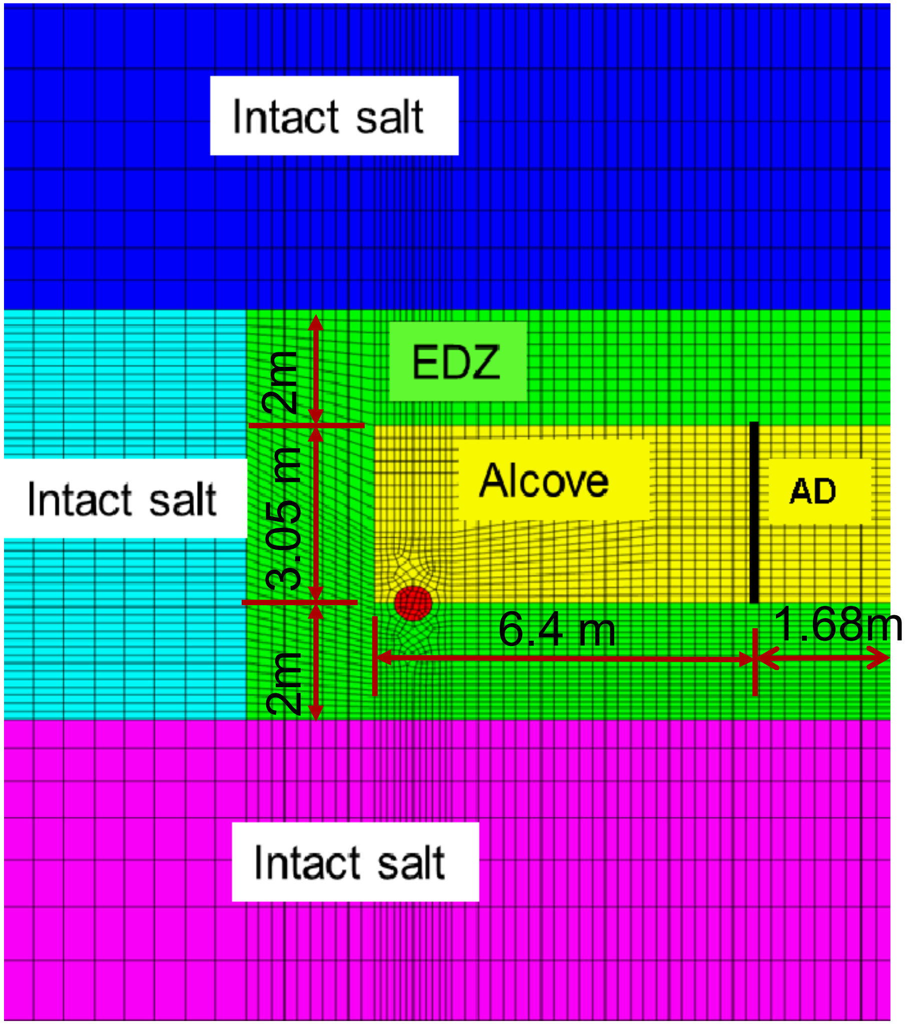
- **Temperatures are used in the constitutive equations for all salt materials (intact and crushed). Pore pressures can be used to compute effective stresses from the total stresses in ADAGIO.**
- **Node displacements from ADAGIO are used to update the ARIA finite element mesh and crushed salt porosity. Thermal conductivity and intrinsic permeability of crushed salt backfill can be adjusted to account for change in porosity due to deformation.**

TM and TH Computational Model



- **Starting point was model developed by D. Clayton in FY11**
- **A EDZ region added to model to account for enhanced permeability due to excavation induced damage. The constitutive models in our codes do not include damage/healing in their formulation.**
- **Need coupling of crushed salt TH properties with mechanical deformation (*e.g.*, porosity [*Φ*] changes)**

Model Details



Waste package:
2.7 m (9 ft) long
0.61 m (2 ft) diameter
12.2 m (40 ft) from the center of the waste canister to a neighboring waste container

Alcove:
6.4 m (21 ft) long, 3.05 m (10 ft) tall and 3.35m (11 ft) wide. It was assumed that the alcove connects at right angle to the access drift

Access Drift (AD):
3.05 m (10 ft) tall, 3.35 m (11 ft) wide access drift.

Constitutive Model for Intact and Crushed Salt

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- Developed by Gary Callahan at RESPEC for modeling shaft seals at WIPP

- A continuum representation of micro-scale and pore scale processes

- Two types of creep behavior

  - Multimechanism Deformation Model (Munson and Dawson) represents dislocation creep behavior and is active for both intact and crushed salt. Uses Tresca equivalent stress.

  - Grain boundary diffusional pressure solution creep (modified Spiers and Brzesowsky) active in crushed salt when moisture is present. Active only when the density of the salt is less than that of intact salt.

Thermal properties for crushed salt

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Thermal conductivity based on Bambus II (Bechtold)

$$\lambda_{c-salt}\left(T\right) = k_{cs}(\phi)\left(\frac{300}{T}\right)^{\gamma}$$

$$k_{cs}(\phi) = \left(-270\,\phi^{4} + 370\,\phi^{3} - 136\,\phi^{2} + 1.5\,\phi + 5\right)\cdot f$$

γ = material constant = 1.4

T = temperature [K]

f = scale factor = 5.4/5.0

ε^{T} = thermal expansion constant = 4.5×10^{-5} K^{-1}

C_s = specific heat = 931 J/Kg-K

ρ = density =2160 Kg/m^{3}

TM Model: Boundary and Initial Conditions

- **Mechanical BC and IC**
  - No lateral displacement on vertical external boundaries of mesh implies an array of alcoves.
  - Bottom boundary- no vertical displacement
  - Top boundary above alcove- applied pressure represents overburden
  - Initial stress varies linearly with depth and at the alcove elevation is 14.8 Mpa

- **Thermal BC and IC**
  - No heat transfer across vertical external boundaries of the mesh
  - Constant temperature maintained on top and bottom
  - Initial temperature throughout mesh is constant at 25 ^{o}C
  - Heat source is 2 kW with decaying half-life of ~26.5 years

- Moisture content in crushed salt is constant in all TM calculations

Average Backfill Porosity vs. Time

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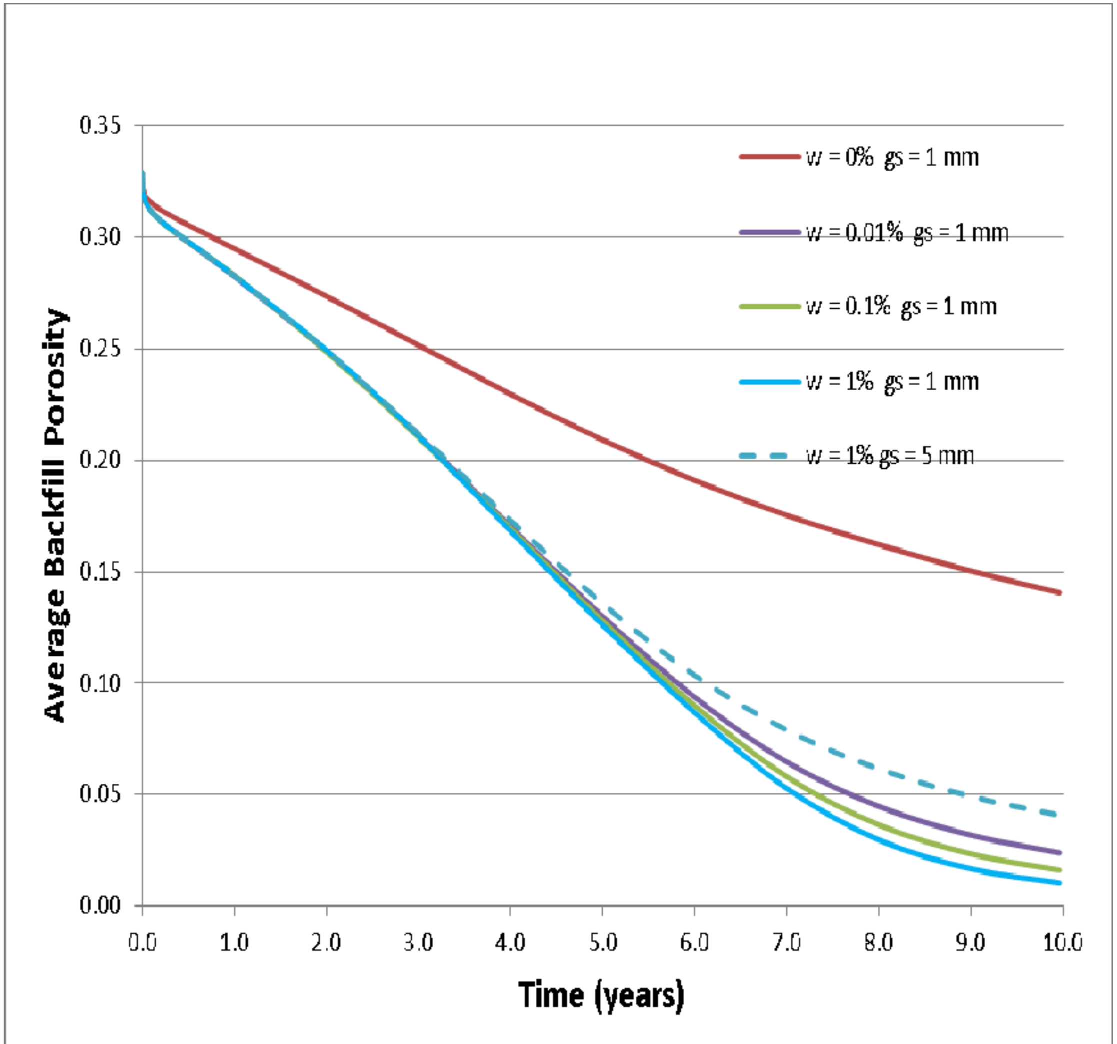
Influence of water content (w) and grain size (gs)



Model Inputs :

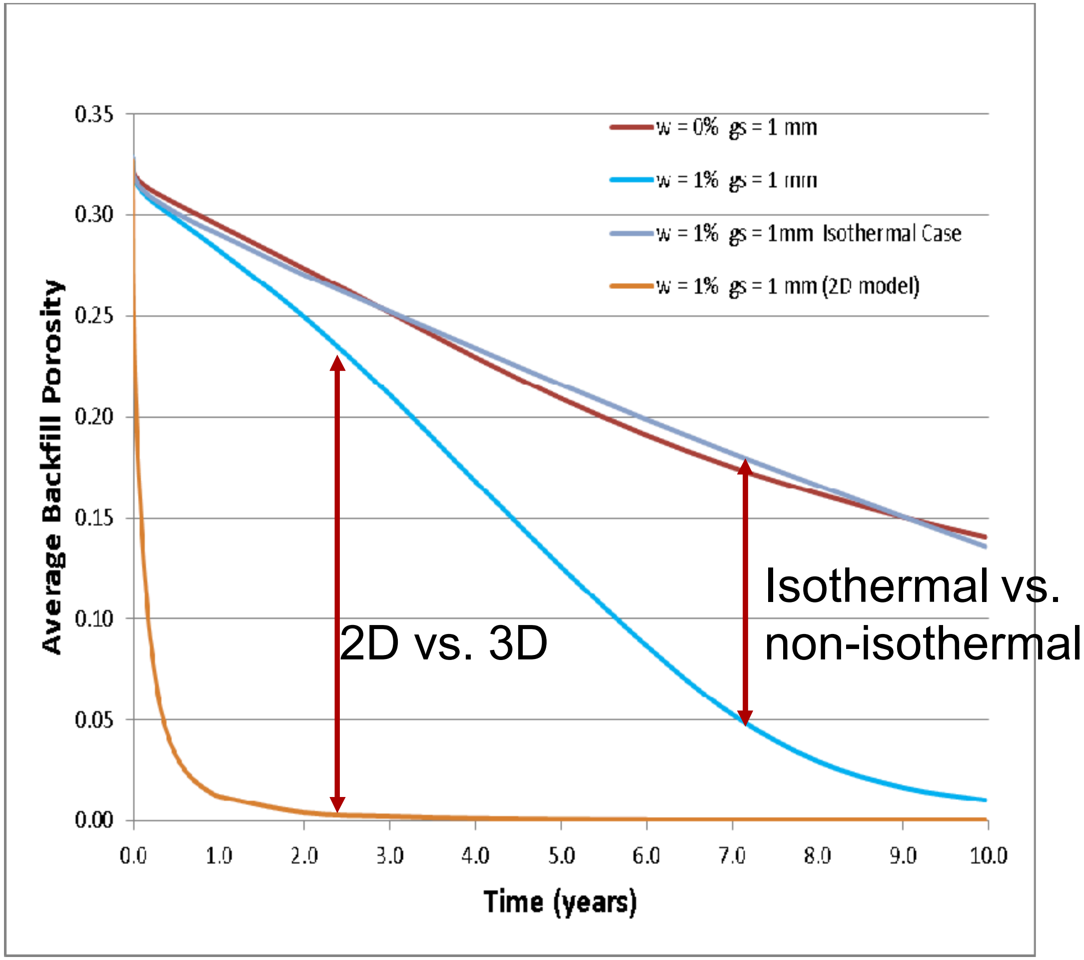
- **Water content varied (0, 0.01% , 0.1% and 1%)**
- **Unless noted all results are for grain size (gs) = 1 mm**

Simulation Results:

- **After about 4 years, crushed salt backfill provides less resistance to creep of surrounding rock as the water content is increased.**
- **Increasing grain size increases time to reach a target backfill consolidation**

Average Backfill Porosity vs. Time

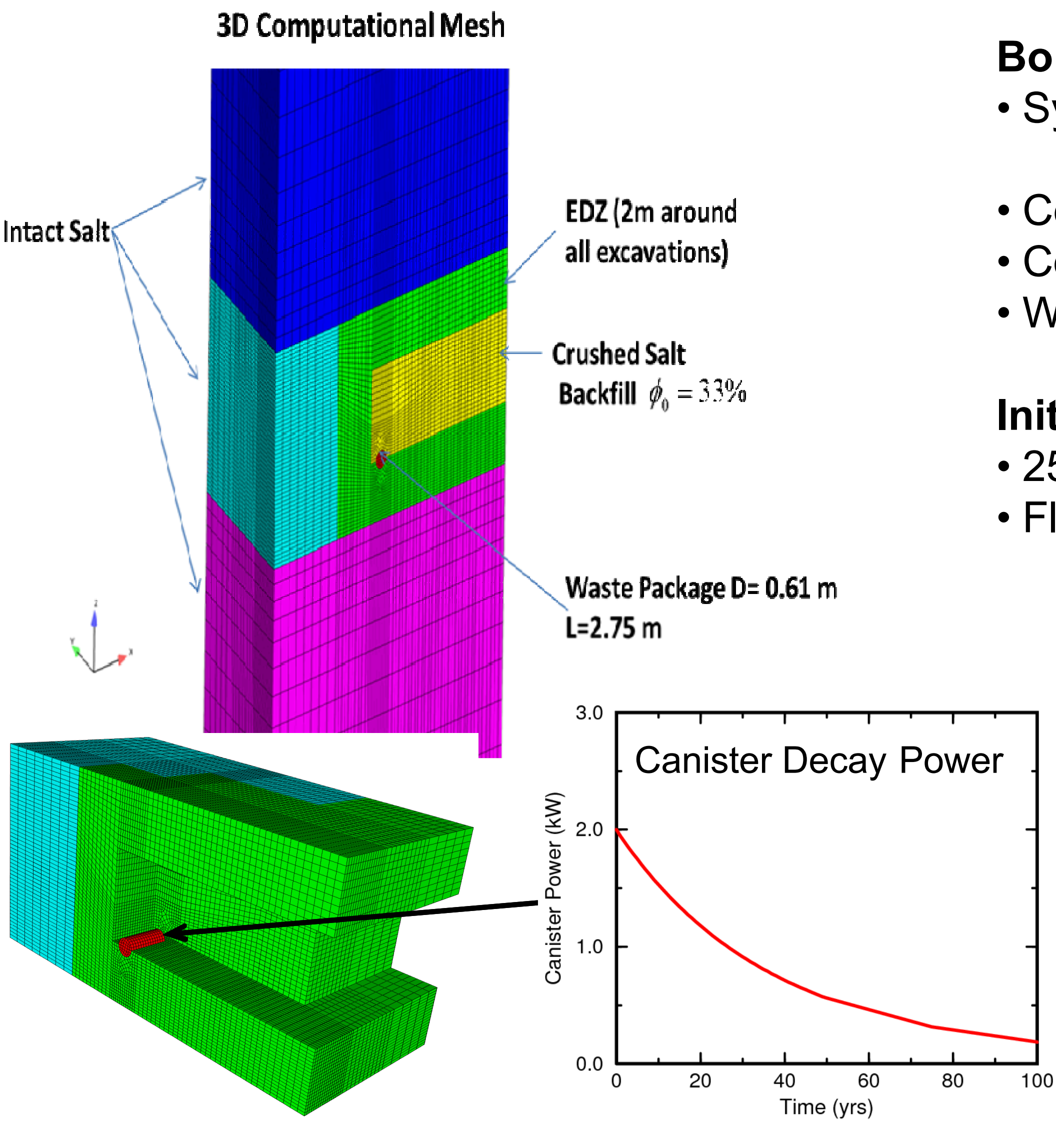
Influence of thermal effects and 2D-3D model geometry



2D Model ignores the pillars between the alcoves resulting in rapid consolidation of excavated regions.

Isothermal simulation gives closure history very similar to the non-isothermal dry crushed salt backfill case.

Thermo-Hydrologic Simulation:
Geometry, Boundary & Initial Conditions

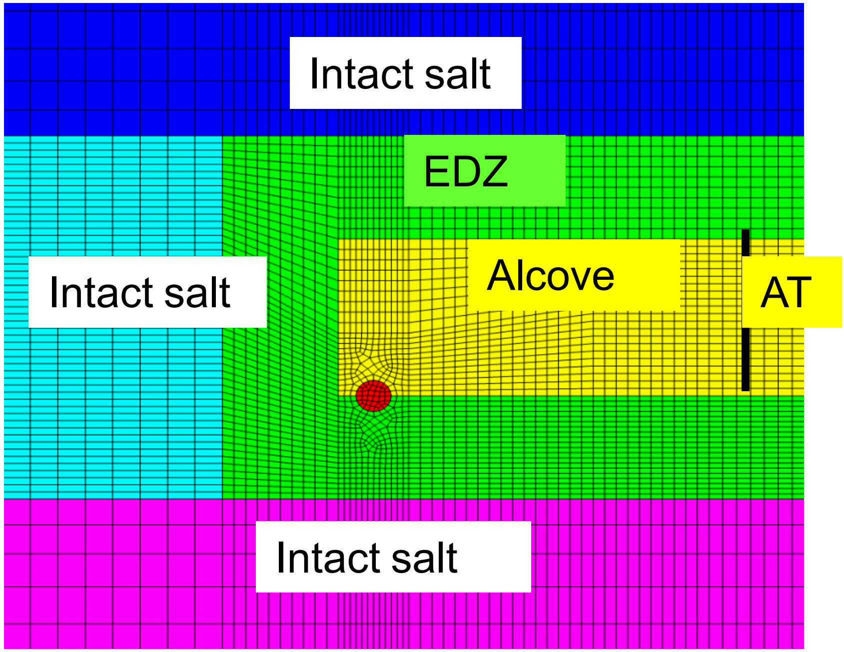


Boundary Conditions:
- Symmetry on lateral (vertical) boundaries
    - insulated (*i.e.*, adiabatic), no-flow
- Constant T top & bottom
- Constant P top, no-flow bottom
- Waste canister: solid, volumetrically heated

Initial Conditions:
- 25 ^{o}C
- Fluid Saturation
    - EDZ: 50% saturation (0.7% moisture)
    - Backfill: 4% saturation (1.3% moisture)

Properties

Property	Intact Salt	EDZ Salt	Crushed Salt	Waste Package
Porosity	0.01	0.014	0.35	-
Permeability (m^2)	10^{-21}	10^{-17}	10^{-13}	-
Saturation, liquid-residual; S_{lr}	0.05	0.05	0.01	
Grain density (kg/m^3)	2190	2190	2190	2200
Specific heat (J/kg K)	931	931	931	840
Thermal Conductivity (W/m K)	5	5	1	2



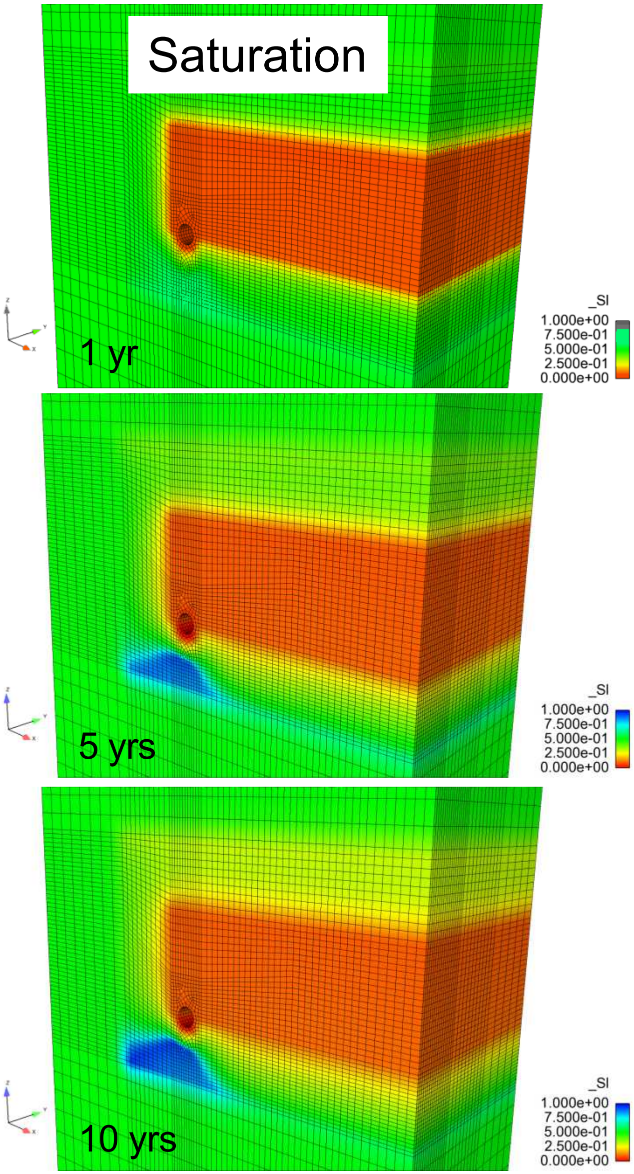
Relative permeability & capillary pressure

$$k_{rl} = s^3 \qquad k_{rg} = (1-s)^3$$

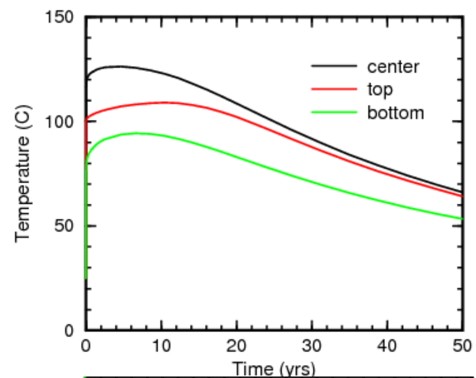
$$p_c = p_{c0}\left(s^{-1/\lambda} - 1\right)^{1/\beta} \qquad \lambda = 1 - 1/\beta$$

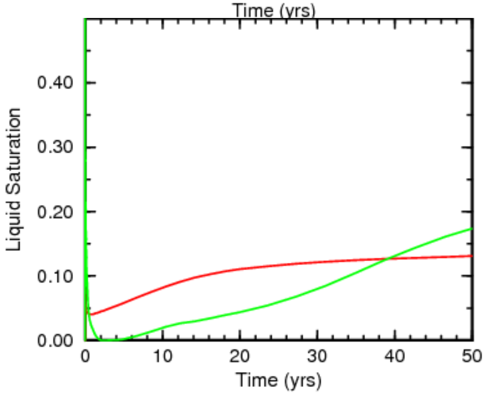
$$s = (S_l - S_{lr}) / ((1 - S_{gr}) - S_{lr})$$

Temperature and Saturation

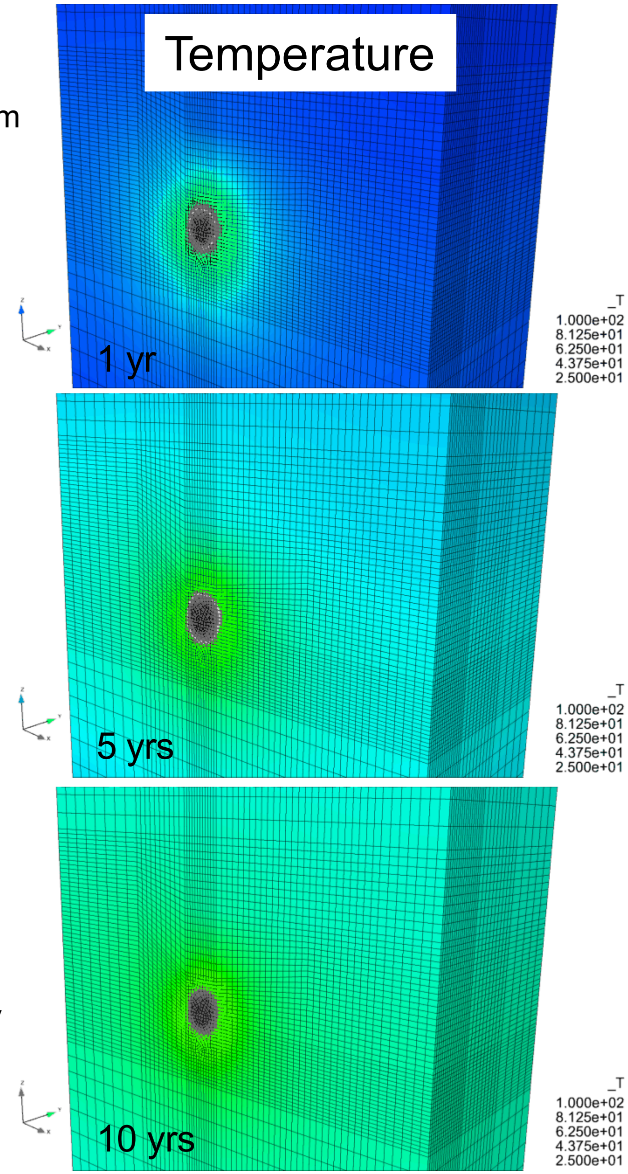


• canister T > 100 ºC at one year
• decay heat drives EDZ moisture away from canister via pressure gradient





• Elevated temperatures at 10 years
• EDZ moisture trapped by low permeability intact salt
• EDZ dewatering



Observations on Moisture Transport (uncoupled from mechanics)

- Decay heat evaporates liquid moisture at the canister, creating a region of high vapor concentration and elevated gas pressure near the canister

- Pressure pushes vapor and liquid from canister, creating near-canister dry-out (no-liquid) regions in EDZ

- Moisture is trapped below canister by ultra-low intact salt permeability (1 nano-Darcy)

Future Work

- Coupled flow and mechanics (THM)
  - Strain-dependent transport properties (ϕ(strain), k(ϕ), λ(ϕ), …)
  - Pore-pressure effects (resists consolidation?)
  - Moisture effects on crushed salt consolidation included in a spatially and time dependent manner
- Numerical issues with coupling large-strain reconsolidation?
  - Investigate coupling strategies
- Need to introduce damage effects (dilation) in salt constitutive models as in German models
- Funding to continue moving forward and future international collaborations?

Backup Slides

Crushed Salt Model Equations

total creep strain rate

$$\dot{\varepsilon}_{ij}^{c} = \dot{\varepsilon}_{ij}^{d} + \dot{\varepsilon}_{ij}^{w}$$

dislocation creep strain rate

$$\dot{\varepsilon}_{ij}^{d} = \dot{\varepsilon}_{eq}^{d}\left(\sigma_{eq}^{f}, T\right)\frac{\partial \sigma_{eq}}{\partial \sigma_{ij}}$$

pressure solution creep strain rate

$$\dot{\varepsilon}_{ij}^{w} = \dot{\varepsilon}_{eq}^{w}\left(\sigma_{eq}^{f}, T\right)\frac{\partial \sigma_{eq}}{\partial \sigma_{ij}}$$

equivalent stress measures

$$\sigma_{eq}^{f} = \sigma_{eq}^{f}\left(\sigma_{m}, \sigma_{T}, D\right)$$

$$\sigma_{eq} = \sigma_{eq}\left(\sigma_{m}, \sigma_{T}, D\right)$$

σ_m = mean stress

σ_T = maximum principal stress difference = $\sigma_1 - \sigma_3$

D = fractional density = 1 - porosity

Kinetic Equations for Dislocation Creep

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$$\dot{\varepsilon}_{eq}^{d} = F\dot{\varepsilon}_{s} = F\sum_{i=1}^{3}\dot{\varepsilon}_{s_i}$$

F accounts for primary or transient creep

Three dislocation mechanisms in the model

1st mechanism: $$\dot{\varepsilon}_{s_1} = A_1\left(\frac{\sigma_{eq}^{f}}{\mu}\right)^{n_1} e^{-\frac{Q_1}{RT}}$$

These are secondary or steady state creep terms

2nd mechanism: $$\dot{\varepsilon}_{s_2} = A_2\left(\frac{\sigma_{eq}^{f}}{\mu}\right)^{n_2} e^{-\frac{Q_2}{RT}}$$

All dislocation creep mechanisms are temperature and stress dependent

3rd mechanism: $$\dot{\varepsilon}_{s_3} = \left(B_1 e^{-Q_1/RT} + B_2 e^{-Q_2/RT}\right)\sinh\left[q\left(\frac{\sigma_{eq}^{f}-\sigma_0}{\mu}\right)\right]H\left(\sigma_{eq}^{f}-\sigma_0\right)$$

The first mechanism (dislocation climb) dominates at low equivalent stress and high temperature. The second mechanism dominates at low stress and temperature. The third mechanism (dislocation slip) is predominately active at high stress for all temperatures.

Kinetic Equation for Pressure Solution Creep

$$\dot{\varepsilon}_{eq}^{w} = \frac{r_1 w^a}{d^p} e^{-\bar{\varepsilon}_v} \left(\frac{e^{r_3 \bar{\varepsilon}_v}}{\left| e^{\bar{\varepsilon}_v} - 1 \right|^{r_4}} \right) \frac{e^{-\frac{Q_s}{RT}}}{T} \Gamma \sigma_{eq}^{f}$$

r_1, r_3, r_4, Q_s, a, p	material constants
T	absolute temperature
R	universal gas constant
d	salt grain size
w	moisure fraction by weight
$\bar{\varepsilon}_v$	volumetric strain
Γ	geometry function

Note that if the crushed salt is dry (w=0), the pressure solution contribution to the total strain rate vanishes. As porosity goes to zero the value of the geometry function also goes to zero.

Organization of Presentation

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- **Sierra Mechanics Physics Coupling Strategy**
- **Thermal- Mechanical (TM) Modeling**
  - **Briefly describe the constitutive model for intact and crushed salt**
  - **Results- Focus on consolidation time of the crushed salt backfill for varying values of assumed moisture content**
- **Thermal-Hydraulic (TH) Modeling**
  - **Model moisture movement due to decay heat in the crushed salt and EDZ regions**
- **Summary and Future Work**

Aria Porous Flow Physics

Two-Phase Heat and Mass Flow

Mathematical Model

- Two-Phase Component Mass and Energy Balances:

$$\frac{\partial}{\partial t}\begin{bmatrix} \phi\left(S_l\rho_l^w + S_g\rho_g^w\right) \\ \phi\left(S_l\rho_l^a + S_g\rho_g^a\right) \\ (1-\phi)\rho_s e_s + \phi\left(\rho_l S_l e_l + \rho_g S_g e_g\right) \end{bmatrix} + \nabla\bullet\begin{bmatrix} \mathbf{F}_l^w + \mathbf{F}_g^w \\ \mathbf{F}_l^a + \mathbf{F}_g^a \\ \mathbf{q}_e \end{bmatrix} + \begin{bmatrix} Q_w \\ Q_a \\ Q_e \end{bmatrix} \begin{matrix} \textbf{water} \\ \textbf{air} \\ \textbf{energy} \end{matrix}$$

- **Net Mass Flux:**

$$\mathbf{F}_\beta^\alpha = Y_\beta^\alpha \rho_\beta \mathbf{v}_\beta + \mathbf{J}_\beta^\alpha$$

$$\alpha = \text{component}$$

$$\beta = \text{phase}$$

- **Darcy Velocity:**

$$\mathbf{v}_\beta = -\frac{k_{r\beta}}{\mu_\beta}\mathbf{k}\bullet\left(\nabla P_\beta - \rho_\beta \mathbf{g}\right)$$

- **Binary Diffusion (gas phase):**

$$\mathbf{J}_g^\alpha = -\rho_g D_g^\alpha \nabla Y_g^\alpha$$

Aria Porous Flow Physics

Two-Phase Heat and Mass Flow

Mathematical Model (cont.)

- Total Energy Flux (heat conduction, convection, binary diffusion):

$$\mathbf{q}_e = -\lambda_T \nabla T + \sum_\beta \rho_\beta \mathbf{v}_\beta h_\beta + \sum_\alpha h_g^\alpha \mathbf{J}_g^\alpha$$

- **Saturation Constraint:** $S_l + S_g = 1$
- **Mixing Rules:** $\sum_{\beta=l,g} Y_\beta^\alpha = 1, \quad \alpha = w\,(\text{water}),\, a\,(\text{air})$
- **Capillary Pressure:** $P_g - P_l = P_c(S_l)$
- **Relative Permeability:** $k_{r,\beta} = f(S_l, T, \ldots)$