Revisiting Historic Numerical Analyses of the Waste Isolation Pilot Plant (WIPP) Room B and D \textit{in-situ} Experiments Regarding Thermal and Structural Response

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Abstract

This report documents several numerical analyses simulating the isothermal and thermal-mechanical (TM) response of the Waste Isolation Pilot Plant (WIPP) Room B and Room D in-situ experiments that were conducted during the late 1980s. This work was funded by the Used Fuels Disposition (UFD) Campaign during the Fiscal Year (FY) 2012. Isothermal, thermal-mechanical uncoupled, and thermal-mechanical coupled calculations simulating the WIPP experiments were conducted using the state-of-the-art Sandia Integrated Environment for Robust Research Algorithms (SIERRA) solid and thermal mechanics computer codes. These calculations used a high-fidelity constitutive law that mathematically describes the multi-mechanism deformation (MD) creep processes inherent to those found in nuclear waste repository environment. Both the WIPP Room D (isothermal) and Room B (heated) numerical models are presented in detail, and results from these numerical calculations are compared to historic numerical calculations and to experimentally measured data.
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1. INTRODUCTION

This report describes the application of the SIERRA Mechanics code suite to a set of nuclear waste repository problems and to demonstrate its use on anticipated more complex coupled simulations involving potential future salt-type nuclear waste repositories. The SIERRA Mechanics code suite is well suited to address the following problems of interest:

- The simulation of the WIPP Overtest for Simulated Defense High-Level Waste (Room B) Thermal/Structural Interactions in-situ experiment (D. E. Munson, 1990);
- Thermal-hydrologic-chemical-mechanical-biological-radiologic coupled physics and/or any subset of these coupled physics related to simulating the near and far-field response of underground nuclear waste repositories.

Results from the various simulations will be presented and discussed to illustrate the capabilities available in SIERRA Mechanics for simulating salt repositories thermal and/or structural/thermal response. These simulations, i.e., numerical calculations, will exercise the SIERRA Mechanics code suite (i.e., a toolset) in a validation exercise against known existing ambient and elevated temperature Waste Isolation Pilot Plant (WIPP) room response data as represented by two well documented WIPP Thermal/Structural Interactions (TSI) experimental rooms for which high-quality data on their response was gathered and is available. While such a comparison between legacy tools and data has been performed in the 1980’s and 1990’s, the modern SIERRA Mechanics toolset has never been exercised against the existing data. In addition, comparisons with historical validation calculations with the earlier legacy codes will also be made to see what can be learned from those earlier calculations that might allow for improvements in future analyses that may be subject to even closer scrutiny than ever before during the licensing process in any future regulatory environment.

The development of the SIERRA Mechanics code suite has been funded by the Department of Energy (DOE) Advanced Simulation and Computing (ASC) program for more than ten years. The goal is development of massively parallel multi-physics capabilities to support the Sandia engineering sciences mission. SIERRA Mechanics was designed and developed from its inception to run on the latest, most sophisticated, massively parallel computing hardware. It has the capability to span the hardware range from a single workstation to computer systems with thousands of processors. The foundation of SIERRA Mechanics is the SIERRA toolkit, which provides finite element application-code services such as: (1) mesh and field data management, both parallel and distributed; (2) transfer operators for mapping field variables from one mechanics application to another; (3) a solution controller for code coupling; and (4) included third party libraries (e.g., solver libraries, communications package, etc.). The SIERRA Mechanics code suite is comprised of application codes that address specific physics regimes. The two SIERRA Mechanics codes that are used as the launching point for fully integrated Thermal Mechanical (TM) coupling, with adaptive solution control, in a repository-setting are Aria (Notz, et al., 2007) and Adagio (Team, 2010). The physics currently supported by Aria include: the incompressible Navier-Stokes equations, energy transport equation, and species transport equations, as well as generalized scalar, vector, and tensor transport equations. A multi-phase porous flow capability has been recently added to Aria. Aria also has basic geochemistry functionality available through embedded chemistry packages. The solid mechanics portion of the TM coupling is handled by Adagio. It solves quasi-static, large deformation, large strain behavior of nonlinear solids in three dimensions. Adagio has Sandia-
developed (i.e., proprietary) technology for solving solid mechanics problems, that involves matrix-free iterative solution algorithms for efficient solution of extremely large and highly nonlinear problems. This advanced technology is especially well-suited for scalable implementation on massively parallel computers. The TM coupling is done through a solution controller within the SIERRA Mechanics called Arpeggio.

The WIPP Room D and Room B TSI in-situ test configurations and the computational models that were used in this work are described herein. - Rooms B and Room D were chosen because they were located in the same general location within the WIPP and at the same horizon, with the major difference between them being that Room D was at ambient conditions while Room B was subjected to a significant thermal load via heaters in the floor (representative of Defense High Level Waste [DHLW]).

This report documents the SIERRA Mechanics code calculations of the isothermal WIPP Room D response, and heated WIPP Room B in-situ response (uncoupled mechanics), and three heated WIPP Room B in-situ response (fully-coupled mechanics) calculations. All of these SIERRA Mechanics code results are compared to historic numerical calculations, and to experimental data. Section 2 describes the constitutive law used in the numerical calculations modeling isothermal and non-isothermal salt creep. Section 3 presents the isothermal room SIERRA Mechanics code calculation (WIPP Room D). Section 4 presents the uncoupled SIERRA Mechanics code calculations. Lastly, Section 5 presents the fully-coupled SIERRA Mechanics code calculations.
2. A MULTI-PHYSICS CONSTITUTIVE LAW FOR SALT

This section focuses on a constitutive model appropriate for analyzing the performance of underground repositories that ultimately provide permanent storage of nuclear waste materials. The tunnel (i.e., a room) and a representative extent of material, including other geologic strata, above and below the excavation, any backfill, and a representation of the waste packages are typically modeled in a high-fidelity model with a 3D high-resolution mesh to capture the heterogeneity of the materials in the room and surrounding rock (e.g., overburden, potential disturbed rock zone [DRZ], and/or near field). Constitutive models are needed to capture detailed spatial and temporal evolution of deformation and heat transfer in the room. A detailed gap analysis report of Wang et al. (Wang, et al., 2011) has recommended building the next generation of "fully coupled high-fidelity codes" for modeling nuclear waste repository behavior on the SIERRA platform for the following reasons:

- The development of the SIERRA Mechanics code suite (SIERRA: A Software Environment for Developing Complex Multi-Physics Applications, 2001) has been funded by the DOE Advanced Scientific Computing (ASC) program for over ten years, with the goal being the development of massively parallel multi-physics capabilities to support the Sandia engineering sciences mission;

- SIERRA Mechanics was designed and developed to run on the latest and most sophisticated massively parallel computing hardware; spanning the hardware computing space from a single workstation to computer systems with 1000's of processors; and

- Recent additional investments in the SIERRA Mechanics code suite have supplied the basic building blocks for realizing this multi-physics capability for repository systems engineering.

- The SIERRA Mechanics approach of coupling thermal and solid mechanics codes, i.e., Aria and Adagio, respectively, does not completely satisfy the "fully-coupled" definition recommended by Wang et al. (Wang, et al., 2011). The SIERRA Mechanics method of coupling these two physics codes may be more accurately described as "loose-coupling".

Several large-scale in-situ tests were fielded underground at the WIPP during the early phase of its development. The expressed purpose of these in-situ tests was to provide the database for validation of the predictive technology that was being developed at the time for use in the licensing process (Matalucci, 1982). Among the pieces of the validation technology being developed then was the Multi-mechanism Deformation (MD) creep constitutive model that was eventually adopted by WIPP. This rock salt constitutive model has seen wide-spread use in waste disposal applications in the U.S. It was originally developed by Munson and Dawson (Munson, et al., 1979), (Munson, et al., 1982), and (Salt Constitutive Modeling using Mechanism Maps., 1984), and later extended by Munson et al., 1989 (Munson, et al., 1989). As mentioned, it was the model of choice for the WIPP licensing application analyses and was originally implemented in the legacy 2D and 3D analytical tools of that time, e.g., SPECTROM-32 (Callahan, et al., 1986), SANTOS (Stone, 1990), and JAC3D (Biffle, 1993), that were used in those historical analyses. This MD model, which has been migrated to (and is available in) the current SIERRA Mechanics toolset, is described in the subsequent sub-section.
2.1. Governing Equations

For mechanical (e.g., geo-mechanical) systems, there are three basic sets of equations that govern the description of a system deforming under a given load. The first set is the equations of motion:

\[ \sigma_{ij,j} + \rho b_j = \rho a_j \]  \hspace{1cm} (2-1)

or for the case when the processes are very slow such that inertia (\( \rho a_j \)), may be neglected, these equations become the equilibrium equations:

\[ \sigma_{ij,j} + f_i = 0 \]  \hspace{1cm} (2-2)

where \( \sigma_{ij} \) are the components of the stress tensor and \( f_i = \rho b_i \) are the body forces, with \( \rho \) being the density. The second set is the set of strain-displacement relations:

\[ e_{ij} = \frac{1}{2} \left( u_{i,j} + u_{j,i} + u_{k,j} u_{k,i} \right) \]  \hspace{1cm} (2-3)

where \( e_{ij} \) is the strain tensor and \( u_i \) is the displacement vector.

The third set of equations, the so-called constitutive equations, relates the equilibrium equations to the strain-displacement relations through the material (constituent) response of the material that is undergoing the deformations. This third set of equations can take on many forms depending on the material that is being modeled, ranging all the way from a simple elastic material that could be used to model, say a granitic material, to materials such as clay and rock salt, with significantly more complicated behaviors that require significantly more sophisticated and involved material descriptions.

As mentioned previously, for the present work, a constitutive model for rock salt is necessary to capture the repository response. Salt is one of many materials of interest for geologic repository performance (Wang, et al., 2011) applications and is a creeping material with a creep rate, \( \dot{\varepsilon}_{ij}^c \), that is highly temperature-dependent. Its overall strain rate can be characterized by the equation:

\[ \dot{e}_{ij} = -\frac{\nu}{E} \dot{\sigma}_{kk} \delta_{ij} + \frac{1+\nu}{E} \dot{\sigma}_{ij} + \dot{\varepsilon}_{ij}^c + 3\alpha \dot{T} \delta_{ij} \]  \hspace{1cm} (2-4)

where \( \nu \) is the Poisson’s ratio, \( E \) is Young’s Modulus, \( T \) is temperature (Kelvin), \( \alpha \) is the coefficient of linear thermal expansion, and \( \delta_{ij} \) is the Kronecker Delta. The temperature is supplied by either a function or by including the loosely coupled physics, via SIERRA thermal mechanics (e.g., Aria), that solves the heat conduction equation, shown in Eq. (2-5)

\[ T = \left( k/(\dot{c}_p \cdot \rho) \right) \nabla T \]  \hspace{1cm} (2-5)
where $k$, $c_p$, and $\rho$, are the thermal conductivity, specific heat capacity at constant pressure, and density, respectively, and $\Delta$ is the Laplace operator.

The MD model mathematically represents the primary and secondary creep behavior of salt due to dislocations under relatively low temperatures (compared to the melting temperature) and low-to-moderate stresses which are typical of mining and storage cavern operations. Three micromechanical mechanisms, determined from deformation mechanism maps (Munson, 1979), are represented in the model: 1) a dislocation climb mechanism active at high temperatures and low stresses, 2) an empirically observed but undefined mechanism active at low temperatures and low stresses, and 3) a dislocation slip (glide) mechanism active at high stresses. This micromechanical mechanism map (Munson, 1979) is shown in Figure 2-1, and these mechanisms are labeled as 3, 5, and 2, respectively. These creep mechanisms are assumed to act such that the total steady state creep rate $\dot{\varepsilon}_s$ can be written as the sum of the individual mechanism strain rates.

$$\dot{\varepsilon}_s = \sum_{i=1}^{3} \dot{\varepsilon}_{s_i} \quad (2-6)$$

The influence of temperature on the creep strain rate is included through an Arrhenius term. The steady state creep strain rates for the first and second mechanisms are identical in form and are implemented using a power law model while the third mechanism (dislocation slip) is represented using an Eyring type model.

$$\dot{\varepsilon}_{s_1} = A_1 \left( \frac{\sigma_{eq}}{G} \right)^{n_1} e^{-\frac{Q_1}{RT}} \quad (2-7)$$

$$\dot{\varepsilon}_{s_2} = A_2 \left( \frac{\sigma_{eq}}{G} \right)^{n_2} e^{-\frac{Q_2}{RT}} \quad (2-8)$$

$$\dot{\varepsilon}_{s_1} = \left( B_1 e^{-\frac{Q_1}{RT}} + B_2 e^{-\frac{Q_2}{RT}} \right) \sinh \left[ q \left( \frac{\sigma_{eq} - \sigma_0}{G} \right) \right] H \left( \sigma_{eq} - \sigma_0 \right) \quad (2-9)$$
Figure 2-1 Deformation Mechanism Map for Salt (Munson, 1979)

where:

\[ \sigma_{eq} \] = equivalent stress
\[ A_i \] and \[ B_i \] = structure factors
\[ Q_i \] = activation energies
\( T = \) absolute temperature  
\( G = \) shear modulus  
\( R = \) universal gas constant  
\( n_i = \) stress exponents  
\( q = \) stress constant  
\( \sigma_0 = \) stress limit of the dislocation slip mechanism  
\( |H| = \) Heaviside function with the argument \( (\sigma_{eq} - \sigma_0) \)

The third creep mechanism, shown in Eq. (2-9), is only active when the equivalent stress exceeds the specified value of the stress limit \( \sigma_0 \), by definition of the Heaviside function. The equivalent stress appearing in these equations is taken to be the Tresca stress (Munson, et al., 1989). The Tresca stress can be written in terms of the maximum and minimum principal stresses \( \sigma_1 \) and \( \sigma_3 \) respectively \( (\sigma_1 \geq \sigma_2 \geq \sigma_3) \). Alternatively, the Tresca stress may be written as a function of the Lode angle \( \psi \) and the second invariant \( J_2 \) of the deviatoric stress tensor \( \mathbf{s} \) (whose components are \( s_{ij} \)).

\[
\sigma_{eq} = \sigma_1 - \sigma_3 = 2 \cos \psi \sqrt{J_2} \tag{2-10}
\]

The Lode angle is dependent on both the second and third invariant \( J_3 \) of the deviatoric stress tensor \( s_{ij} \).

\[
\psi = \frac{1}{3} \sin^{-1} \left[ \frac{-3 \sqrt{3} J_3}{2 J_2^{3/2}} \right] \quad -\frac{\pi}{6} \leq \psi \leq \frac{\pi}{6} \tag{2-11}
\]

\[
J_2 = \frac{1}{2} s_{ij} s_{ij} \tag{2-12}
\]

\[
J_3 = \frac{1}{3} s_{ij} s_{jk} s_{ki} \tag{2-13}
\]

The transient creep is incorporated into the MD model using the function form given by Eq. (2-15) where \( F \) is a function which accounts for transient creep effects and \( \dot{\varepsilon}_s \) is the steady state dislocation creep strain rate defined by Eq. (2-6).

\[
\dot{\varepsilon}_{eq} = F \dot{\varepsilon}_s \tag{2-14}
\]

The function \( F \) has three branches: a work hardening branch \( (F > 1) \), an equilibrium branch \( (F = 1) \), and a recovery branch \( (F < 1) \), as shown in Eq. (2-15).
The choice of the particular branch depends on the transient strain limit, $\varepsilon_i^{\prime}$, and the internal variable, $\zeta$. The transient strain limit is defined by Eq. (2-16) where $K_o$, $c$, and $m$ are material parameters, $T$ is the absolute temperature, and $G$ is the shear modulus.

$$\varepsilon_i^{\prime} = K_o e^{c T} \left( \frac{\sigma_{eq}}{G} \right)^m \quad (2-16)$$

The internal variable, $\zeta$, appearing in the calculation of the function, $F$, is obtained by integration of the evolution equation

$$\dot{\zeta} = (F - 1) \dot{\varepsilon}_i \quad (2-17)$$

$\Delta$ and $\delta$, appearing in Eq. (2-17), are the work hardening and recovery parameters and are given by Eqs. (2-18) and (2-19), respectively. In these equations $\alpha$, $\beta$, $\alpha_r$, and $\beta_r$ are material parameters. Typically the recovery parameter $\delta$ is taken to be constant (i.e., $\delta = \alpha_r$).

$$\Delta = \alpha + \beta \log \left( \frac{\sigma_{eq}}{G} \right) \quad (2-18)$$

$$\delta = \alpha_r + \beta_r \log \left( \frac{\sigma_{eq}}{G} \right) \quad (2-19)$$

For three dimensional states of stress the components of the creep strain rate tensor are generalized (Fossum, et al., 1988) as

$$\dot{\varepsilon}_{ij}^{eq} = \dot{\varepsilon}_{eq} \frac{\partial \sigma_{eq}}{\partial \sigma_{ij}} \quad (2-20)$$

Using the Tresca stress, Eq. (2-10), as the equivalent stress in this form means the creep strains are purely deviatoric ($\dot{\varepsilon}_{ij}^{eq} = \dot{\varepsilon}_i^{eq}$ since $\dot{\varepsilon}_{kk}^{eq} = 0$) and that all volume change is elastic as defined though the bulk modulus $K$ (i.e., $\varepsilon_{kk} = \frac{\sigma_{kk}}{3K}$). Therefore Eq. (2-20) becomes
\[ \dot{\varepsilon}_{ij}^c = \dot{\varepsilon}_{eq} \frac{\partial \sigma_{eq}}{\partial \sigma_{ij}} = \dot{\varepsilon}_{eq} N_{ij} \quad (2-21) \]

Including the bulk and shear moduli, which are both assumed constant, there are a total of 19 parameters used to define the MD model.
3. UNHEATED ROOM CALCULATIONS (WIPP ROOM D)

3.1. Test description and stratigraphy

The isothermal WIPP Mining Development Test (Room D) consists of a test room set into the bedded stratigraphy of the natural salt formation. The room was constructed to be thermally and structurally isolated from the other test rooms by a large pillar, approximately 79 m thick. The room has a total length of 93.3 m. The test section of the room consists of the central 74.4 m of the room and has cross sectional dimensions of 5.5 m wide by 5.5 m high. The Room D coordinate center is at a depth of 646.0 m below the ground surface. Details of the mining of the room and of the measurements that were taken are given by Munson et al., 1988 (Munson, et al., 1988). The roof of Room D follows a parting defined by a small clay seam. This seam (Clay I), along with the rest of the clay seams, and the remainder of the stratigraphy around the room are shown in Figure 3-1. This is the same stratigraphy used in the historical calculation of Munson et al., 1989 (Munson, et al., 1989), in which they reported agreement of the MD-model/SPECTROM-32 (2D) code combination with the Room D data. In this work, the authors attempted to duplicate the published closure results from the historical calculation, shown in Figure 3-2, as closely as possible with the MD-model/SIERRA toolset combination as an initial effort at validating SIERRA Mechanics for this class of problems.
Figure 3-1 Local stratigraphy around and model of Room D.
The clay seams noted in the stratigraphy, according to Munson et al., 1989 (Munson, et al., 1989), are not in actuality distinct seams unless associated with an anhydrite layer but are rather local horizontal concentrations of disseminated clay stringers. Therefore, seam properties can be ascribed to the concentration of clay, and incorporated into calculations using computational contact surfaces. In the calculational model of this work, as was also the case for the historical calculation, the clay seam shear response is specified by a coefficient of friction, $\mu$, equal to a value of 0.2. Although there are thirteen clay seams labeled A through M, only the nine nearest the room, labeled D through L, are considered active and included in the calculation.

### 3.2. Configuration and computational model

The numerical model represents a slice through the center of the room length and consists of a space defined by the vertical symmetry plane through the middle of the room and by a vertical
The problem involves the modeling of stress and displacement in a room placed in a salt formation. The model is a plane strain model, which is appropriate for comparison with measurements taken at room mid-length for the relatively long room. Because the SIERRA mechanics toolset offers only a 3D capability, for the room calculations reported herein, the plane strain model is approximated by taking a slice (single element into the plane) to generate its 3D equivalent. The front and back faces of the resulting 3D model are then constrained against movement in the out-of-plane direction (Z-direction). The upper and lower extremes of the model are defined as shown. The boundaries, both vertical and horizontal, are sufficiently removed from the room that they cause an insignificant perturbation in stress or displacement at the room proper. Both of the vertical boundaries are constrained against horizontal (X-direction in Figure 3-1) movement, allowing only vertical displacements.

The horizontal boundaries are traction (i.e., lithostatic pressure) boundaries. A uniform pressure of 13.57 MPa is applied at the upper horizontal boundary, accounting for the weight of the overburden. Krieg (Krieg, 1984) determined the thickness weighted average of the densities of the materials in the layers of the numerical model yielding an average density in the model of 2.30 Mg/m$^3$. This density results in a uniform applied pressure of 15.97 MPa on the bottom horizontal boundary, and accounts for the presence of an instantaneously-mined room.

A lithostatic initial stress state that varies linearly with depth is assumed, based on the average material density and a gravitational acceleration of 9.79 m/sec$^2$, in the model. The room surfaces are traction-free and the upper right corner of the numerical model is fixed against horizontal and vertical (X-Y in Figure 3-1) displacements, and is also fixed in the out-of-plane (i.e., Z-direction) displacements.

The overall finite element mesh used in the SIERRA Mechanics calculation used in the Room D calculation is shown in Figure 3-3, and a close-up in the vicinity of the room is shown in Figure 3-4. It contains 2184 hexahedral elements and 5032 nodes and represents a mesh refinement that, the authors believe, is comparable to that used in the historical calculation because of the computer resources available at the time. However Munson et al., 1989 (Munson, et al., 1989) did not show a mesh for the historical calculation, so there is some uncertainty in the mesh that was used for the historical calculation. Because this was a preliminary validation effort that was constrained by time and budget, there was no additional refinement of the mesh attempted for Room D. Such a mesh refinement study would certainly need to be an activity performed in a more complete validation effort. Target tolerances of the both the code and the constitutive model were some of the things that were investigated and adjusted to insure that the MD Model in SIERRA Mechanics was providing an accurate solution.
Figure 3-3 Overall mesh used for the SIERRA Mechanics Room D simulation.
3.3. Closure results from SIERRA Mechanics

The Room D simulation computed the first 1100 days of creep response of the room for comparison with the Room D measurements. The simulation used the above-described computational model and MD constitutive description, with the parameters for the MD model shown in Table 3-1. Again in an effort to duplicate, as closely as possible, the historical calculation using SIERRA Mechanics, in place of the earlier 2D SPECTROM-32 code, these parameters are identical to those given in Munson et al., 1989 (Munson, et al., 1989). Only a few of the parameters shown in Table 3-1 are different between clean halite (labeled “Salt”) and argillaceous halite (labeled “Arg. Salt”); most parameters are the same for the two materials that were used in the calculation.
Table 3-1 Material properties of salt used in the SIERRA Mechanics Room D analysis

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Salt</th>
<th>Arg. Salt</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Elastic Properties</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Shear modulus</td>
<td>$G$ MPa</td>
<td>12,400</td>
<td>12,400</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>$E$ MPa</td>
<td>31,000</td>
<td>31,000</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$\nu$</td>
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<td>0.25</td>
</tr>
<tr>
<td><strong>Salt Creep Properties</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Structure Factors</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A_1$ s$^{-1}$</td>
<td></td>
<td>8.386×10$^{22}$</td>
<td>1.407×10$^{23}$</td>
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<tr>
<td>$B_1$</td>
<td></td>
<td>6.086×10$^6$</td>
<td>8.998×10$^6$</td>
</tr>
<tr>
<td>$A_2$</td>
<td></td>
<td>9.672×10$^{12}$</td>
<td>1.314×10$^{13}$</td>
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<tr>
<td>$B_2$</td>
<td></td>
<td>3.034×10$^{-2}$</td>
<td>4.289×10$^{-2}$</td>
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<tr>
<td>Activation energies</td>
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<td>25,000</td>
<td>25,000</td>
</tr>
<tr>
<td></td>
<td>$Q_2$ cal/mole</td>
<td>10,000</td>
<td>10,000</td>
</tr>
<tr>
<td>Universal gas constant</td>
<td>$R$ cal/mol-K</td>
<td>1.987</td>
<td>1.987</td>
</tr>
<tr>
<td>Absolute temperature</td>
<td>$T$ K</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>Stress exponents</td>
<td>$n_1$</td>
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<td>5.5</td>
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<tr>
<td></td>
<td>$n_2$</td>
<td>5.0</td>
<td>5.0</td>
</tr>
<tr>
<td>Stress limit of the dislocation slip mechanism</td>
<td>$\sigma_0$ MPa</td>
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<td>20.57</td>
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<tr>
<td>Stress constant</td>
<td>$q$</td>
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<td>5.335</td>
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<tr>
<td>Transient strain limit constants</td>
<td>$M$</td>
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<td>3.0</td>
</tr>
<tr>
<td></td>
<td>$K_0$</td>
<td>6.275×10$^6$</td>
<td>2.470×10$^6$</td>
</tr>
<tr>
<td></td>
<td>$c$ K$^{-1}$</td>
<td>9.198×10$^{-3}$</td>
<td>9.198×10$^{-3}$</td>
</tr>
<tr>
<td>Constants for work-hardening parameter</td>
<td>$\alpha$</td>
<td>-17.37</td>
<td>-14.96</td>
</tr>
<tr>
<td></td>
<td>$\beta$</td>
<td>-7.738</td>
<td>-7.738</td>
</tr>
<tr>
<td>Recovery parameter</td>
<td>$\delta$</td>
<td>0.58</td>
<td>0.58</td>
</tr>
</tbody>
</table>

Thus, it should be noted that the same assumptions that went into the historical calculation were also used in this one. For example, although the stratigraphy shows anhydrite and polyhalite layers, Munson et al., 1989 (Munson, et al., 1989) state: “Because these layers are either sufficiently thin to be insignificant in the calculational response or are sufficiently removed from the room being simulated to be quite un-influential in the calculational response, we did not include them in the calculation.” Hence, the present SIERRA mechanics calculation did not include them either; instead the two materials were treated as argillaceous halite as was presumably done in the historical calculation. It should also be noted that not all of the details of
the historical calculations are well-documented, as was the case of refinement of the mesh. Therefore, in those cases where those details are missing, the authors have made some assumptions, guided by their experience, to repeat the historical calculation as closely as possible. Such was the case in treating the anhydrite and polyhalite layers as argillaceous halite rather than clean halite.

Figure 3-5 shows the room closure results from the SIERRA Mechanics simulation compared to the extensometer measurements of the Room D closure. The “data,” shown in this figure, were obtained by digitizing that information from Figure 3-2. Note that this problem contains numerous non-linearities, including both transient and secondary salt creep response in addition to multiple contacting surfaces. The numerical treatment of contact surfaces, controls and manages whether or not two surfaces, each defined by either an analytic representation or a collection of finite element faces, have interpenetrated. In view of the complexity of the calculation, the agreement between calculation and measurement is quite good, on the order of approximately 10% difference between them for both vertical and horizontal closure. This is of roughly the same order as the agreement seen in the historical calculation of Munson et al., 1989 (Munson, et al., 1989), and at least, in a preliminary sense, validates SIERRA Mechanics for isothermal conditions to roughly the same degree as was done for the code used in the historical calculation. The SIERRA Mechanics simulation was stopped after 1100 days since it over-predicted both the vertical and horizontal response closure response. One explanation of this over-predicted closure response may be pointed at the clay seam friction value of 0.2. Historically, this value has been interrogated, demonstrating that values ranging from 0.4 to 0.2 result a change in vertical closure of 10% and a change in horizontal closure of about 5% (Munson, et al., 1989). Also, all clay seams are homogenous in the numerical treatment of contact surfaces; that is, there is no variance in friction value with regard to each clay seam. A complete listing of the Adagio code input deck used in all unheated room structural simulations is provided in Appendix A.
Figure 3-5 Comparison of computed (SIERRA Mechanics) and measured in-situ Room D closure response.
4. HEATED ROOM UNCOUPLED CALCULATIONS (WIPP ROOM B)

The heated room uncoupled simulations are a series of calculations invoking the modern computational tools within the SIERRA analysis suite to simulate thermal and structural response. In particular, the SIERRA codes *Aria* (Notz, et al., 2007) and *Adagio* (Team, 2010) employ thermal and structural response solutions, respectively, that the Sandia National Laboratories (SNL) legacy codes, COYOTE and SANCHO provided many years ago. These heated room uncoupled simulations using Aria and Adagio are based on identical models described by Morgan and Stone 1985 (Morgan, et al., 1985) in the pretest reference calculations for the experiment simulating the response of buried defense high level waste (*i.e.*, the WIPP Room B *in-situ* Experiment). A slight variation in the modeling efforts was allowed to permit the best stratigraphic representation of the geologic layers surrounding the WIPP Room B, which was provided by Munson 1997 (Munson, 1997). Thus, the stratigraphic representation of the geologic layers surrounding the WIPP Room B was chosen identical to that shown in Figure 3-1 (isothermal WIPP Room D configuration).

The Waste Isolation Pilot Plant (WIPP) overtest for simulated Defense High Level Waste (DHLW) or the Room B experiment, was a thermally overdriven, isolated room similar to rooms planned for actual DHLW tests in 1989 (Matalucci, et al., 1982). Resistance heaters were placed in the floor and uniformly spaced along the length of the room to provide a thermal load approximately four times greater than the areal load typically associated with DHLW. The location of Room B, shown in plan view in Figure 4-1, is 93 3 m (306 ft) long with an overtest
heater section of 24.4 m (80 ft) in the central portion of the room. The overtest heaters have power levels of 1.8 kW and a center-to-center spacing of 1.524 m (5 ft). Guard heaters and other heaters designed to resemble DHLW canisters are located at the extremities of the central heater array to insure uniform temperature distributions along the entire length of the test section. The WIPP Room B is 5.49 m (18 ft) wide and 5.49 m (18 ft) high as shown in Figure 4-2. The
overtest heaters are placed in boreholes, 4.877 m (16 ft) long and 0.406 m (16 in) in diameter, which have been drilled in the center of the floor.

Figure 4-2 Details of Canister Emplacement for the WIPP Room B

The heaters are 0.305 m (12 in) in diameter and 3.048 m (10 ft) long. However, heat is produced only in the bottom 2.59 m (8.5 ft) section of the canisters. The floor of WIPP Room B is located...
1.08 m (3.5 ft) below the reference zero defined in the WIPP reference stratigraphy (Kreig, et al., 1982). This corresponds to a depth of approximately 651.53 m (2137.6 ft) beneath the ground surface at the WIPP. The WIPP Room B experiment consists of two phases: (1) a six month period between the time when excavation was completed and the time when the heaters were turned on, and (2) and the following three years when heat was supplied to the room. The heating schedule was constructed to conform with the decay pattern in common DHLW having a thirty year half-life. The WIPP Room B heaters were activated 324 days after the excavation start date (March 23, 1985 i.e., Julian day 5113) according to Munson, et.al 1990 (Munson, et al., 1990). Thus, the Aria thermal simulations incorporated 324 days of unheated operations

4.1. Heated room uncoupled model

The finite element calculations used to simulate the WIPP Room B experiment consisted of two separate three-dimensional models, a thermal model and a structural model. One-way coupling between the thermal and structural responses was employed, similar to what was performed using the SNL legacy codes COYOTE and SANCHO (or the RESPEC Codes SPECTROM-41 and SPECTROM-32 used in the historical calculations). This one-way coupling implies that thermal response was assumed to be unaffected by structural deformations. The thermal model was used to compute temperatures in the geologic formation around the Room B excavation (i.e., opening) for a simulated period of five years. The thermal mechanics code, Aria (Notz, et al., 2007) was used for this calculation. The temperatures were then used as input to the mechanics code, Adagio (Team, 2010) so that thermal expansion and creep property changes induced by changes in temperature could be included in the mechanical response. Since temperature and stress gradients occur in different areas, the thermal and structural calculations required mesh refinement in different areas. As a result, the thermal and structural finite element meshes used for the Room B calculation were different, and nodal temperatures computed using the Aria calculation were interpolated to the nodes of the structural mesh. The interpolation code MAPVAR (Wellman, 1999) was used to perform this task. Thus, the interpolated temperature field is available at the beginning of the Adagio calculation, and the constitutive laws that require temperature (e.g., the MD model) use this information directly during the solution.

A planar representation (i.e., x-y plane) of the WIPP Room B configuration was shown previously in Error! Reference source not found.Error! Reference source not found.. Due to the symmetry of the Overtest experiment, the left boundary (at x = 0), represents a symmetry plane running through the center of the room. Since Room B was considered to be a single isolated room, the location of the right boundary was chosen to be remote enough to preclude its affecting either the thermal or structural response of the room. A distance of 50 m (164 ft) from the left symmetry plane was determined to be an appropriate location for the right boundary based on an earlier computational study (Miller, 1981). The original simulations performed using the legacy codes employed a true two dimensional mesh or grid to capture the thermal and structural response assuming the behavior of an infinitely long, out-of-plane direction (i.e., the z-direction). This assumption corresponds to a plane strain condition for the structural calculation. In order to emulate this similar constraint using the modern SIERRA codes, which are designed primarily for three-dimensional analyses, a pseudo two dimensional grid can be realized using a three dimensional mesh with one element in the out-of-plane direction and appropriate boundary conditions to enforce a plane strain condition. This method (one-element z-direction thickness model) was applied to three dimensional finite element models used in simulations presented in this report.

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4.2. Heated room thermal model

The thermal model was constructed assuming all boundaries were adiabatic, except the Room B boundaries, and that the entire formation was prescribed to have a constant initial temperature of 300 K (i.e., there was no temperature dependence based upon depth beneath the ground level). The configuration remained at 300 K for six months of simulation time. Then the thermal load of 1.8 kW per canister was applied to the finite element model at the appropriate location. The discrete thermal loading from each of the canisters was simulated two-dimensionally as a uniform line source located on the left symmetry plane, extending from a depth of 3.37 m (11.06 ft) below Clay G to a distance of 5.96 m (19.55 ft) below Clay G. The load for each canister was smeared over the canister spacing of 1.524 m (5 ft) and canister height of 2.59 m (8.5 ft) to give a uniform heat flux of 456 W/m² condition on the symmetry plane, only half of this load or 228 W/m² was applied to the thermal finite element model. A thirty year half-life was simulated as a decaying exponential so the thermal load applied along the length of the heat source had the form

\[ q = 228^* \exp(-7 \times 10^{-10}^*t) \]  

(4-1)

where \( q \) is the thermal load in W/m² and \( t \) is the time in seconds. The thermal properties of all stratigraphic materials were assumed to be the same as those for halite. This assumption, which simplified the meshing for the thermal calculation, was appropriate because earlier calculations by Stone (Stone, 1983) had shown that thermal responses computed with an all salt stratigraphy and with a layered stratigraphy were essentially the same. Heat transfer through the salt was modeled with a nonlinear thermal conductivity of the form

\[ \lambda = \lambda_{300} (300/T)^\gamma \]  

(4-2)

where \( \lambda \) is the thermal conductivity, \( T \) is the absolute temperature in Kelvin (K), and \( \lambda_{300} \) and \( \gamma \) are material constants. The excavated room area (i.e., WIPP Room B) was treated as an "equivalent thermal material" with a conductivity allowing radiation heat transfer in the room to be simulated by conduction. This method of modeling radiation was used in the WIPP Benchmark II numerical simulation activity (Morgan, et al., 1981) and (George, 1984), and the properties of the "equivalent thermal material" were chosen so that the thermal response computed with this material is almost the same as the response computed by modeling radiation in the room. Note that the "equivalent thermal material" was not used in the structural model mesh. The thermal properties of halite and the Equivalent Thermal Material (ETM), used in this simulation effort are presented in Table 4-1.

<table>
<thead>
<tr>
<th>Material</th>
<th>Density, ( \rho ) (kg/m³)</th>
<th>Specific Heat, ( C_p ) (J/kg/K)</th>
<th>Thermal Conductivity Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Halite</td>
<td>2300.0</td>
<td>860.0</td>
<td>( \lambda_{300} ) (W/m/K)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>\gamma</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.14</td>
</tr>
</tbody>
</table>
The halite property values were taken from the WIPP reference properties report (Krieg, 1984) and the properties for the "equivalent thermal material" are the same as those used in Benchmark II (Morgan, et al., 1981). Lastly, the thermal loss from the room was modeled by a convective boundary at the WIPP room B surfaces using Newton's law of cooling as:

$$q' \cdot n = h \cdot (T - 300) \quad (4-3)$$

where $q'$ is the thermal flux vector, $n$ is the outward normal unit vector, $h$ is the convective heat transfer coefficient, and $T$ is the surface temperature in Kelvin. The convective boundary acts as a heat sink whenever the temperature on the room surface exceeds the initial 300 Kelvin temperature. Thus, as the room surface temperature rises, the rate of heat loss increases. Because the convective heat transfer coefficient was unknown, it was adjusted prior to any structural calculations until a suitable value (0.18 W/m²/K) was determined to give agreement with the measured temperatures reported above and below the WIPP Room B at gages B_744 and B_745 respectively. Previous numerical calculations performed by Munson, et al. 1990 (Munson, et al., 1990), using the heat transfer code SPECTROM-41 (Svalstad, 1989), determined that a heat transfer coefficient of 0.51 W/m²/K was sufficient to match the collected WIPP Room B test thermocouple B_744 and B_745 test data (Munson, et al., 1990). The SPECTROM-41 thermal simulations predicted temperatures at WIPP Room B thermocouple B_745 locations are shown in Figure 4-3 and compared to the test data and the Aria thermal simulated temperatures. Likewise, Figure 4-4 shows the SPECTROM-41 and Aria thermal simulation predicted temperatures (and test data collected at thermocouple B_744) at locations beneath the floor of Room B.
Figure 4-3 SPECTROM-41 Thermal Simulation (above) and Aria Thermal Simulation (below) Compared with Room B Thermocouple B_745 locations
Figure 4-4 SPECTROM-41 Thermal Simulation (above) and Aria Thermal Simulation (below) Compared with Room B Thermocouple B_744 locations.
The Aria finite element mesh for the WIPP Room B calculation is shown in Figure 4-5 and Figure 4-6 and consists of a 3-dimensional model comprised of eight-node, isoparametric, hexahedral elements. The mesh is comprised of 14110 nodes and 6888 hexahedral elements and is one element thick in the out of plane direction (Z-direction) with $\Delta Z_{\text{element}} = 1.54$ m. Shown in Figure 4-7 is the zoomed-in display of the computational mesh, showing the detail of the elements in the excavated room. Shown in Figure 4-8 is where the DHLW canisters’ simulated heat flux was applied (shown in Magenta, and labeled as SIDE SETS ID 6666) and the thermal convection boundary location of the natural convection heat flux condition, from Eq. (4-3) (shown in Blue, and labeled as NODE SETS ID 400).
Figure 4-6 Aria Three Dimensional 8-node Hexahedral Finite Element Mesh used in Thermal simulations

Figure 4-7 Zoomed in Detail of Aria 3D Finite Element Mesh Near Room B Location (shown in red)
Comparison of the Aria computed temperatures and test recorded thermocouple temperatures at gage B 706 are shown in Figure 4-9. Shown in Table 4-2 are the tabulated comparisons of the test and simulation temperatures at gage B 706 at 1200 days. Predicted near field temperature contours of Room B using both a coarse thermal mesh (consisting of 1276 nodes and 588 elements and is one element thick in the out of plane direction with $\Delta Z_{\text{element}} = 1.54 \text{ m}$) and the reference thermal mesh, shown previously in Figure 4-5 (containing 14110 nodes and 6888 elements), are presented for various times in Figure 4-10 and Figure 4-11, respectively. As seen in these figures, after the thermal load is applied (at 200 days or 0.55 years) the temperature contours expand radially from the center of the heaters with some alteration due to influence of the Room B and the convection heat loss boundary condition. The coarse mesh and reference mesh temperature response is virtually the same. These temperature contour plots reflect lower temperature response compared with those predicted temperature contours derived by the COYOTE simulations and documented by Morgan and Stone, 1985 (Morgan, et al., 1985), and may indicate a different treatment of the thermal convection boundary condition between the Aria and COYOTE simulations. This difference in thermal response, i.e., COYOTE vs Aria, may also be due in part to 2-dimensional 9-noded quadrilateral elements (being higher order element type [COYOTE]) and the use of single point integration 3-dimensional 8-noded hexahedral elements utilized in the Aria simulations.
Figure 4-9 Measured temperatures at thermocouple Unit B 706 (top) and comparison of Aria predicted temperatures with measured temperatures (bottom).
Table 4-2 Tabulated Comparisons of Simulated Temperatures to Thermocouple Temperatures at gage B_706 at 1200 years.

<table>
<thead>
<tr>
<th>Room B Thermocouple Unit B_706 ID</th>
<th>Aria Simulation Thermocouple Location ID</th>
<th>Vertical Distance from Room B Center (m)</th>
<th>Vertical Distance from Room B Floor (m)</th>
<th>Thermocouple Temperature at 1200 days (°C)</th>
<th>Aria Simulated Temperature at Thermocouple Location at 1200 days (°C)</th>
<th>Difference Between Experiment and Simulation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>F7</td>
<td>16.72</td>
<td>15.2</td>
<td>45</td>
<td>48</td>
<td>7</td>
</tr>
<tr>
<td>2</td>
<td>F6</td>
<td>11.11</td>
<td>9.2</td>
<td>60</td>
<td>61</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>F5</td>
<td>7.15</td>
<td>4.9</td>
<td>85</td>
<td>87</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>F4</td>
<td>4.35</td>
<td>1.8</td>
<td>90</td>
<td>89</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>F3</td>
<td>3.49</td>
<td>0.9</td>
<td>75</td>
<td>77</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>F2</td>
<td>3.22</td>
<td>0.6</td>
<td>80</td>
<td>72</td>
<td>10</td>
</tr>
</tbody>
</table>

In general, the comparison of temperatures predicted by Aria and compared to the temperatures measured at thermocouple locations at Unit B 706, shown in Figure 4-9, are reasonable with respect to the uncertainty of the equivalent thermal material model property values. One metric for measuring the quality of the numerical predictions, as seen in Table 4-2, displays the difference in experiment and simulated temperatures is at most 10%. A complete listing of the Aria code input deck used in the heated room uncoupled thermal simulation is provided in Appendix B.
Figure 4-10 Coarse Thermal Mesh Computed Temperature Contours Drawn over Coarse Structural Deformed Mesh at Time = 0, 1, 2, 3, 4, and 5 years.
Figure 4-11 Reference Thermal Mesh Computed Temperature Contours Drawn over Reference Structural Deformed Mesh at Time = 0, 1, 2, 3, 4, and 5 years.
4.3. Heated room structural model

In the structural model, horizontal displacements were constrained to be zero on the left symmetry plane and on the right boundary as shown in Error! Reference source not found. Error! Reference source not found.. The vertical displacements were constrained to be zero along the right boundary at the uppermost anhydrite location, and consistent with the historic calculation by Morgan and Stone (Morgan, et al., 1985). Traction were applied to both the top and bottom boundaries with the top traction representing the load from the overburden above the configuration and the bottom traction representing the sum of the overburden load and the weight of the rock in the configuration. The overburden load was calculated by assuming an average overburden density of 2320 kg/m$^3$. A density of 2300 kg/m$^3$ was used for all stratigraphic layers in assigning body forces representing the weight of the rock and in computing the bottom traction. The traction value of 15.97 MPa, at the bottom boundary, accounts for rock removed from the room area due to excavation. An initial lithostatic stress state which varied linearly with depth, using a ratio of horizontal to vertical stress equal to one, was applied and the room was assumed to appear instantaneously as a void at time $t = 0$ and a gravitational acceleration of $9.79$ m/sec$^2$. The finite element mesh used in the structural calculation is shown in Figure 4-12, and Figure 4-13 shows a zoomed in view near the excavated Room B with several clay seams displayed. The three dimensional reference mesh comprised of eight-node, isoparametric hexahedral elements, used an hourglass stiffness control parameter of 0.003 to prevent undesirable element response, based on geomechanics experience from related analyses. The finite element mesh consisted of 28284 nodes and 13248 elements and is one element thick in the out of plane direction (z-direction) with $\Delta Z_{element} = 0.28$ m. The horizontal mesh spacing was graded so that a large number of elements were near the room where the stress gradients are the highest. The vertical mesh spacing was dictated predominantly by the stratigraphy shown in Error! Reference source not found. Error! Reference source not found.. The stratigraphy consists of layers of five different materials, namely, halite, argillaceous halite, anhydrite, polyhalite, and clay (e.g., clay seams).
Figure 4-12 Heated Room Structural Model Finite Element Mesh
The MD constitutive model was employed in the structural simulations and allowed the thermal affects (i.e., non-isothermal conditions) to be coupled from the thermal simulation to the structural response. The remaining materials, anhydrite and polyhalite, were simulated using a isothermal Drucker-Prager failure criteria constitutive model to treat elastic and inelastic behavior. The mechanical response of the anhydrite and polyhalite materials was assumed to be isotropic and elastic until yielding occurs. Once this yield stress has been achieved, plastic strain can be accumulated. A simple Prager-Drucker failure criterion that represents this behavior can be written as

\[ \sqrt{J'_2} = C - aJ_1 \]  

(4-4)

where \( \sqrt{J'_2} \) is the second deviatoric stress invariant, \( C \) is a constant, and \( J_1 \) is the first stress invariant. The above equation can also be transformed into the form
\[ \bar{\sigma} = \sqrt{3}C + 3\sqrt{3}aP \quad (4-5) \]

or

\[ \bar{\sigma} = a_0 + a_1P \quad (4-6) \]

where \( \bar{\sigma} \) is the von Mises or equivalent stress (and \( \bar{\sigma} = \sqrt{3}\sqrt{J_2} \)), \( P \) is the pressure (negative one third of the trace of the stress tensor), and \( a_0 \) and \( a_1 \) are parameters in the so-called “soil and crushable foam” material model. The Drucker-Prager failure criterion material model is a simplification of the Adagio "soil and crushable foam" material model (Team, 2010) whereby the quadratic pressure term (i.e., \( a_2 \)) is ignored. The soil and crushable foam model is a plasticity model whereby the yield surface is surface revolution about the hydrostat. The halite and argillaceous halite Multi-mechanism deformation creep material parameters used in the Adagio structural simulations are listed in Table 4-3. Similarly, the anhydrite and polyhalite Drucker-Prager material model parameters used in the Adagio structural simulations are presented in Table 4-4.
Table 4-3 Multi-mechanism Deformation Model Parameters for Halite and Argillaceous Halite

<table>
<thead>
<tr>
<th>Creep Parameter</th>
<th>Halite</th>
<th>Argillaceous Halite</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shear Modulus, $G$</td>
<td>$1.249 \times 10^{10}$</td>
<td>$1.24 \times 10^{10}$</td>
<td>Pa</td>
</tr>
<tr>
<td>Poisson Ratio, $\nu$</td>
<td>0.2484221834</td>
<td>0.25</td>
<td>1</td>
</tr>
<tr>
<td>$A_1$</td>
<td>$8.386 \times 10^{22}$</td>
<td>$1.406 \times 10^{25}$</td>
<td>sec$^{-1}$</td>
</tr>
<tr>
<td>$Q_1/R$</td>
<td>12581.78158</td>
<td>12581.78</td>
<td>Kelvin</td>
</tr>
<tr>
<td>$N_1$</td>
<td>5.5</td>
<td>5.5</td>
<td>1</td>
</tr>
<tr>
<td>$B_1$</td>
<td>6086000</td>
<td>8993300</td>
<td>sec$^{-1}$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>$9.672 \times 10^{12}$</td>
<td>$1.313 \times 10^{13}$</td>
<td>sec$^{-1}$</td>
</tr>
<tr>
<td>$Q_2/R$</td>
<td>5032.71</td>
<td>5032.71</td>
<td>Kelvin</td>
</tr>
<tr>
<td>$N_2$</td>
<td>5</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>$B_2$</td>
<td>0.03034</td>
<td>0.042875</td>
<td>sec$^{-1}$</td>
</tr>
<tr>
<td>$\sigma_0$</td>
<td>20570000</td>
<td>20570000</td>
<td>Pa</td>
</tr>
<tr>
<td>$Q_{lc}$</td>
<td>5335</td>
<td>5335</td>
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</tr>
<tr>
<td>$M$</td>
<td>3</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>$K_0$</td>
<td>627500</td>
<td>2470000</td>
<td>1</td>
</tr>
<tr>
<td>$C$</td>
<td>0.009189</td>
<td>0.009189</td>
<td>Kelvin$^{-1}$</td>
</tr>
<tr>
<td>Alpha</td>
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<td>-14.96</td>
<td>1</td>
</tr>
<tr>
<td>Beta</td>
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<td>-7.738</td>
<td>1</td>
</tr>
<tr>
<td>DelatC</td>
<td>0.58</td>
<td>0.58</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Algorithm Parameter</th>
<th>Halite</th>
<th>Argillaceous Halite</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amult</td>
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<td>0.5</td>
<td>1</td>
</tr>
<tr>
<td>Grwfac</td>
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<td>1.05</td>
<td>1</td>
</tr>
<tr>
<td>Esptol</td>
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<td>0.01</td>
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<tr>
<td>Shkfac</td>
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<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Itype</td>
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<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Angle</td>
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<td>0.1</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 4-4 Prager-Drucker Failure Criterion Parameters for Anhydrite and Polyhalite

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Anhydrite</th>
<th>Polyhalite</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic Modulus, $E$</td>
<td>$7.51 \times 10^{10}$</td>
<td>$5.53 \times 10^{10}$</td>
<td>Pa</td>
</tr>
<tr>
<td>Poisson Ratio, $\nu$</td>
<td>0.36</td>
<td>0.36</td>
<td>1</td>
</tr>
<tr>
<td>$C$, Prager-Drucker</td>
<td>$1.35 \times 10^{76}$</td>
<td>$1.42 \times 10^{76}$</td>
<td>Pa</td>
</tr>
<tr>
<td>$a$, Prager-Drucker</td>
<td>0.45</td>
<td>0.473</td>
<td>1</td>
</tr>
<tr>
<td>$a_{00}$, Soil-Crushable Foam</td>
<td>2338268.59</td>
<td>2459512.147</td>
<td>Pa</td>
</tr>
<tr>
<td>$a_{11}$, Soil Crushable Foam</td>
<td>2.33826859</td>
<td>2.45778096</td>
<td>1</td>
</tr>
</tbody>
</table>

Thermal strains were included in the constitutive model by using the thermal strain option in the Adagio code (Team, 2010). The thermal strain functions used for each stratigraphic layer (i.e., polyhalite, argillaceous halite, anhydrite, and halite) was based on a reference temperature, $T_{ref}$, of 300 Kelvin, a maximum temperature, $T_{max}$ of 1500 Kelvin, and a linear coefficient of thermal expansion, $\alpha_T$ as a piecewise linear functions of temperature and strain:

$$T_{ref} \quad \text{Thermal Strain} = 0.0$$
Thermal Strain = \((T_{\text{max}} - T_{\text{ref}}) \times \alpha_T\)

Thus, at any temperature \(T\), between \(T_{\text{ref}}\) and \(T_{\text{max}}\), the thermal strain value is obtained through linear interpolation. Shown in Table 4-5 are the coefficients of linear thermal expansion, \(\alpha_T\) [18], used in all Room B structural simulations.

<table>
<thead>
<tr>
<th>Material</th>
<th>Coefficient of Linear Thermal Expansion, (\alpha_T [\text{Kelvin}^{-1}])</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polyhalite</td>
<td>24.0 (\times) (10^{-6})</td>
</tr>
<tr>
<td>Argillaceous Halite</td>
<td>40.0 (\times) (10^{-6})</td>
</tr>
<tr>
<td>Anhydrite</td>
<td>20.0 (\times) (10^{-6})</td>
</tr>
<tr>
<td>Halite</td>
<td>45.0 (\times) (10^{-6})</td>
</tr>
</tbody>
</table>

There were nine distinct clay seams (clay D through clay L) included in the structural simulations of the heated room calculation. All clay seams were treated as sliding material interfaces and uniquely defined as computational side sets in the finite element model since they were extremely thin in the vertical or y-direction. Thus, each clay seam was represented as a boundary between a block of contiguous material elements which had non-coincident nodes (although duplicate in geometric coordinates) to correctly address sliding friction and contact conditions. Seven of the nine clay seams (clay F through Clay L) can be seen in the finite element mesh shown in Figure 4-13. Also depicted in Figure 4-13 are the reference elevations in meters (m) and the associated computational model sideset identifiers which are used to designate contact and friction interface conditions. The nine clay seams (Clay D, E, F, G, H, I, J, K, and Clay L) are known to have a great effect on room closure response (Stone, et al., 1981). Each of the clay seams was modeled using a dry friction algorithm to describe the slip behavior between layers of material above and below the clay seam interface. The dry friction model employed in the uncoupled heated room structural simulations used a no slip criterion based if the shear stress along the interface is less than \(\mu\), the coefficient of friction, times the normal stress. Otherwise, slip occurs between the two surfaces at the interface, and the shear stress is constrained to be equivalent to \(\mu\) times the normal stress. A coefficient of friction value, \(\mu = 0.2\), was used in all clay seam interactions. The initial stress condition involving tractions of 15.97 MPa at the lower boundary and 13.57 MPa at the upper boundary (vertical or y-direction) of the finite element model invoked at simulation time, \(t = 0\), and is shown in Figure 4-14.
The simulated Room B closure histories are presented in the next three figures. Closure is often used to quantify the deformation of an excavated underground room. Thus, closure will be defined as the sum of the absolute values of displacements of two points on opposite surfaces. In order to compare the closure response, three closure measurements: vertical, horizontal, and rib (or pillar) shortening were obtained during the experiment in Room B. The vertical closure is measured between points A1 and L1 displayed in Figure 4-15; horizontal closure is twice the absolute horizontal displacement of point I1, and pillar shortening is measured between points K1 and G1.
The Room B closure response computed from a SANCHO (Stone, et al., 1985) 2-dimensional
simulation (Morgan, et al., 1985) is shown in Figure 4-16. Similarly, the results of a
SPECTROM-32 code simulation (Munson, et al., 1990) predicting closure response compared
with test data recorded from extensometers placed around the vicinity of Room B (using data from
extensometers A1, G1, K1, and L1) (Munson, et al., 1990) is shown in Figure 4-17. Lastly,
Figure 4-18 and Figure 4-19 display the results from the one-way coupled (i.e., uncoupled) Aria-
Adagio structural simulation prediction of the Room B response (both coarse and Reference
Mesh). In order to accurately compare test data from the extensometers, the thermal simulations
were run using 324 days of unheated operations. Then at day 325, thermal heating was initiated.
(i.e., the heaters were activated on Julian day 5113, nearly 324 days after room excavation and mining operations were began (Munson, et al., 1990) [see page 57]. As seen in Figure 4-18 and Figure 4-19, the Adagio structural simulation predictions of room response are close to the recorded test data and very similar in magnitude to the historic SANCHO and SPECTROM-32 calculations.
Figure 4-16 Room B Closure Response predicted by a SANCHO two dimensional calculation [9].

Figure 4-17 Room B Closure Response predicted by SPECTROM-32 and compared with recorded extensometer test data [19].
Figure 4-18 Room B Closure Response predicted by the uncoupled Heated Room Adagio simulation and compared to recorded extensometer test data (Coarse Mesh).

Figure 4-19 Room B Closure Response predicted by the uncoupled Heated Room Adagio simulation and compared to recorded extensometer test data (Reference Mesh).
Shown in Table 4-6 are the tabulated comparisons of the Room B vertical and horizontal closure response and test data at 1200 days (3.29 years). Based on similar closure results computed from the Adagio simulation, it is a reasonable conclusion that the new code (Adagio) has matched the experiment closure response in the same manner that was demonstrated in the historical calculations of Munson et al., 1990 (Munson, et al., 1990).

Table 4-6 Computed Heated Room Closure Response compared with Extensometer Data at 1200 days

<table>
<thead>
<tr>
<th>Source</th>
<th>Vertical Closure (m)</th>
<th>Horizontal Closure (m)</th>
<th>Difference Between Experiment and Simulation: Vertical Closure (%)</th>
<th>Difference Between Experiment and Simulation: Horizontal Closure (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test Data</td>
<td>0.85</td>
<td>0.46</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>SANCHO</td>
<td>0.60</td>
<td>0.40</td>
<td>29</td>
<td>15</td>
</tr>
<tr>
<td>SPECTROM-32</td>
<td>0.67</td>
<td>0.42</td>
<td>21</td>
<td>11</td>
</tr>
<tr>
<td>Adagio (Coarse mesh)</td>
<td>0.66</td>
<td>0.46</td>
<td>22</td>
<td>0</td>
</tr>
<tr>
<td>Adagio (Reference Mesh)</td>
<td>0.64</td>
<td>0.45</td>
<td>25</td>
<td>2</td>
</tr>
</tbody>
</table>

Predicted deformed shapes of Room B using both a coarse mesh (consisting of 5032 nodes and 2184 elements and is one element thick in the out of plane direction with $\Delta Z_{\text{element}} = 0.45$ m) and the reference mesh, shown previously in Figure 4-12 (containing 28284 nodes and 13248 elements), are presented for various times in Figure 4-20 and Figure 4-21, respectively. As seen in each of these figures, the letters F, G, H, I, and J to the right of the upper left snapshot (at $t = 0$ years) deformed shape denote the corresponding clay seam locations. In both the coarse mesh and reference mesh deformation snapshots, there is considerable slippage along Clay F and Clay J after two years, recognizable by the mesh discontinuities. A complete listing of the Adagio code input deck used in all heated room uncoupled structural simulations is provided in Appendix B.
Figure 4-20 Coarse Mesh Structural Simulation: Deformation vs. Time Snapshots
Figure 4-21 Reference Mesh Structural Simulation: Deformation vs. Time Snapshots
5. HEATED ROOM COUPLED CALCULATIONS (WIPP ROOM B)

The work detailed in the previous two sections (3 & 4) was initiated and mainly performed under the Nuclear Energy Advanced Modeling & Simulation (NEAMS) Waste Integrated Performance and Safety Codes (IPSC) during FY 2011. It constituted a preliminary validation of the SIERRA Mechanics toolset for salt geologic repository applications and was summarized in an article published in the Proceedings of the 7th International Conference on the Mechanical Behavior of Salt (SIERRA Mechanics for Coupled Multi-Physics Modeling of Salt Repositories, 2011). This article, in its entirety, is included in Appendix C. The work of sections 3 and 4 was, however, only a preliminary validation in that it exercised just a subset of the capability available in SIERRA by using limited aspects of the toolset to repeat the one-way coupling procedure that had been used in earlier historical calculations. At the time, funding and time constraints prevented anything beyond that. Fortunately, in FY 2012 the Used Fuels Disposition Campaign, under the FCR&D program, had an interest in the “benchmarking” of computational tools for use in rock salt geologic repositories and, efforts to further validate SIERRA mechanics for this application have been possible. The emphasis of the new UFD benchmark simulations has been two-fold. First and foremost is to demonstrate a truly coupled thermo-mechanical capability. A second emphasis has been an attempt to substitute a more detailed method of capturing the energy transfer with Aria during the thermally active time period in Room B that explicitly better-accounts for heat transfer in the room (i.e., radiation and convection) beyond the pure conduction approximation and “equivalent thermal material” used previously in the historical calculations to account for heat transfer in the room.

The new coupled thermal-mechanical simulations of Room B exercise SIERRA’s coupling capability, using the Arpeggio coupling module in SIERRA. Aria is coupled to Adagio through nodal temperatures, transferring its computed temperature field to Adagio. Adagio accepts the temperature field from Aria and updates its temperature field on its nodes. Adagio is coupled back to Aria through nodal displacements, transferring its computed displacement field to Aria. Aria accepts the displacement field and updates its corresponding nodal coordinates. The Aria and Adagio finite element meshes can be discretized differently to account for different refinement locations. The SIERRA coupling methodology may be further defined as a weakly-coupling approach. A fully coupled thermal-structural code would solve the temperature and displacement fields simultaneously, rather than passing these results from one physics code to another at specific transfer times.

Three coupled numerical models using the SIERRA mechanics coupling controller module, Arpeggio, are presented and the computed results are shown and compared with historic calculations, modern uncoupled calculations, and experimental data in this chapter. The first section is virtually a repeat of the uncoupled heated Room B numerical model and numerical simulation completed in two parts, discussed in section 4 of this report, but now uses the Arpeggio to couple Aria and Adagio to each other. Recall that Section 4 of this report discussed these uncoupled calculations, whereby the Room B air material is represented as an “Equivalent Thermal Material” (ETM). In this first section a similar coupled model, with the air not explicitly represented in the thermal finite element model, is presented and discussed. The second model and numerical calculation include an enclosure radiation boundary condition to simulate radiative heat transfer within the WIPP Room B cavity. The third section presents an alternative boundary condition, Dirichlet temperature applied to the WIPP Room B floor, pillar, and roof, to treat the energy transfer out of the room.
5.1. Heated room coupled model using equivalent thermal material

The thermal finite element model mesh used in the heated room coupled calculations, using the thermal equivalent material, was identical to that shown in Figure 4-6 and Figure 4-7. Similarly, the mechanical finite element model mesh used in the heated room coupled calculations, was the same as shown in Figure 4-12 and Figure 4-13. A brief description of how the SIERRA Mechanics is used to couple the two physics codes, Aria and Adagio, is given in Appendix D.

Three numerical thermal response plots, and one numerical closure response plot, all compared with test data, are shown in Figure 5-1, Figure 5-2, Figure 5-3, and Figure 5-4, respectively. As witnessed in these four comparison response plots, the general trend is that the coupled numerical Arpeggio calculations using the equivalent thermal material resulted nearly identical predictions of the (structural) closure response as those computed with the uncoupled Aria/Adagio calculation (compare Figure 4-19 and Figure 5-4). Also, the thermal response predictions using the coupled Arpeggio equivalent thermal material were virtually the same as the uncoupled Aria/Adagio calculations (discussed earlier in Section 4). This implies (and was expected, based on prior experience) that the coupling between the two physics is dominated by the thermal response. That is, the temperature significantly affects the mechanical deformations, but the deformations, in turn, have a negligible effect on the thermal response. The results from this calculation demonstrate that the coupling feature in SIERRA gives sensible results for this application. A complete listing of the Arpeggio code input deck used in all heated room coupled structural simulations, using the equivalent thermal material, is provided in Appendix E.

![Figure 5-1 Heated Room Coupled Calculation, Using Equivalent Thermal Material, Response Compared To Measured Thermocouple B-706 Temperatures](image-url)
Figure 5-2 Heated Room Coupled Calculation, Using Equivalent Thermal Material, Response Compared To Measured Thermocouple B-745 Temperatures

Figure 5-3 Heated Room Coupled Calculation, Using Equivalent Thermal Material, Response Compared To Measured Thermocouple B-744 Temperatures
Figure 5-4 Heated Room Coupled Calculation, Using Equivalent Thermal Material, Response Compared To Measured Extensometer Data
5.2. Heated room coupled model using enclosure radiation method

This finite element model treated the excavated room B thermal response using enclosure radiation methods which utilize radiative heat transfer at the Room B walls (i.e., floor, pillar, and roof) in contact with air. Again, similar to the previous section, the fully coupled numerical simulations were conducted using Arpeggio, but there was no explicit material representing the air. The thermal mesh used in the enclosure radiation model did not include any material representing the excavated room (i.e., Room B), and is shown in Figure 5-5. A brief description of the SIERRA mechanics operators used in the heated room model using the enclosure radiation method is given in Appendix F. In addition, a few sensitivity calculations were performed using different levels of emissivity, e = 0.3, 0.5, and 1.0, to determine if the predicted temperature field would be raised significantly. Ultimately, neither of these sensitivity calculations produced any heat transfer to the top of the "Room B". Thus with only a small amount energy transfer to the surface (i.e., the top of Room B), there would be only a small increase in temperature, which results insufficient activation of the MD model to deform the surrounding salt.

Three numerical thermal response plots, and one numerical closure response plot, all compared with test data, are shown in Figure 5-6, Figure 5-7, Figure 5-8, and Figure 5-9, respectively. As witnessed in these four comparison response plots, the general trend is that the coupled numerical Arpeggio calculations, using the enclosure radiation method, under-predicted both the thermal and structural (i.e., closure) response when compared to measured data and/or earlier uncoupled calculations. This model appears to be demonstrating that the air material, which is not represented by the thermal model mesh (or the structural mesh), cannot transfer any energy from the excavated room floor surface (directly above the simulated DHLW) to the neighboring pillar and roof surface. The contribution of energy from the radiative heat transfer mechanism appears small, and thus there is only a small increase in temperature, which results in insufficient activation of the creep model to deform the surrounding salt. However, it should be noted that for different waste forms (e.g., High Level Waste and/or Spent Nuclear Fuel), the energy resulting from radiative heat transfer may be more substantial, and thus activate the creep models more significantly.

It is hypothesized that the addition of air in the room and accounting for its circulation via convective heat transfer (in addition to the radiation) may yield the additional heat transfer needed at the roof of the room and the walls to account for the insufficient activation of creep deformation at those locations. Additional study will be required to include the convective heat transfer via an air circulation model.

In summary, the Arpeggio calculations using enclosure radiation under-predict both the thermal and structural response. A complete listing of the Arpeggio code input deck used in all heated room coupled structural simulations, using the enclosure radiation method, is provided in Appendix G.
Figure 5-5 Coupled Room Calculation Thermal Mesh using the Enclosure Radiation Method
Figure 5-6 Heated Room Coupled Calculation, Using Enclosure Radiation, Response Compared To Measured Thermocouple B-706 Temperatures

Figure 5-7 Heated Room Coupled Calculation, Using Enclosure Radiation, Response Compared To Measured Thermocouple B-745 Temperatures
Figure 5-8 Heated Room Coupled Calculation, Using Enclosure Radiation, Response Compared To Measured Thermocouple B-744 Temperatures

Figure 5-9 Coupled Calculation Heated Room Closure, Using Enclosure Radiation, Response Compared To Measured Extensometer Data
5.3. Heated room coupled model using a dirichlet temperature boundary condition

An alternative method, to further probe the question of the importance of the heating contribution from the air in the room, was devised using a Dirichlet temperature model. The Dirichlet temperature model was simply an applied temperature function over several sections of the finite element mesh boundary, in the Room B vicinity. This approach used measured temperature data from the air ventilation Unit B E91 thermocouple gage, see the Appendix from Munson, et al. 1990 (Munson, et al., 1990). The numerical model temperature at the floor used this data directly. The model temperature at the roof used this temperature data plus 5 degrees Celsius, based on Munson, et al. 1990, page 803 (Munson, et al., 1990), which stated: “Although the air in the room is quiescent, a marked vertical gradient causes the air near the roof to be about 5 °C (9 °F) hotter than the air at the floor, as determined by crude manual measurements.” The model temperature at the pillar was linearly interpolated between the floor and roof temperatures based on elevation. Therefore, to incorporate this floor and roof temperature behavior, a "plug-in" file (i.e., a user subroutine) was constructed to implement this constraint on the walls of the room. These prescribed floor and roof temperature histories applied to the computational thermal model are shown in Figure 5-10.

Three numerical thermal response plots, and one numerical closure response plots, all compared with test data are shown in Figure 5-11, Figure 5-12, Figure 5-13, and Figure 5-14, respectively. As can be seen in these response plots, the general trend is that the coupled numerical Arpeggio calculations using the Dirichlet temperature boundary conditions resulted in nearly identical predictions of the (structural) closure response as those computed with the uncoupled Aria/Adagio calculation (compare Figure 4-19 and Figure 5-14). However, the thermal response predictions using the coupled Arpeggio Dirichlet temperature boundary conditions were less than the measured thermocouple temperature data, but slightly improved over the previous calculation, using Arpeggio with the radiation enclosure method, shown in Section 5.2.

Studying Figure 5-13 it can be seen that the predicted temperatures at locations 0.9 and 0.6 m below the room floor (i.e., the Unit 744 B, thermocouple locations directly beneath the Room B floor) are influenced by Dirichlet temperature boundary condition, and thus under-predict the temperature response. If the baseline heated room coupled numerical calculation is chosen as method using the equivalent thermal material (ETM)), then this Dirichlet temperature boundary condition influence can be seen comparing Figure 5-4 with Figure 5-13.

Similarly, comparing and investigating computed temperature response above the room floor, there is a boundary condition influence. Closely examining Figure 5-12, it can be seen that the predicted temperatures at distances 0.6, 0.9, and 1.8 m above the room roof (i.e., Unit 745 B, thermocouple locations directly above the Room B roof) are affected by the Dirichlet temperature boundary condition, and thus over-predict the temperature response. Again, if the baseline heated room coupled numerical calculation is chosen as the method using ETM, then this Dirichlet temperature boundary condition influence can be seen comparing Figure 5-3 with Figure 5-12.

A general conclusion that can be drawn from these results is that incorporating the air in the room and correctly capturing its thermal response throughout the room should lead to a better prediction of both thermal and mechanical responses in a configuration that does not use a conductive “equivalent thermal material” alone. A complete listing of the Arpeggio code input
deck and user "plug-in" file (i.e., a user subroutine, t_dirich3.C) used in all heated room coupled structural simulations, using the Dirichlet temperature boundary condition, is provided in Appendix H.

![Diagram](image)

**Figure 5-10** Dirichlet Temperature Boundary Condition Model and Measured Thermocouple B-E91 Temperature (model=red and green; data=blue)
Figure 5-11 Heated Room Coupled Calculation, Using Dirichlet Temperature Boundary Condition, Response Compared To Measured Thermocouple B-706 Temperatures

Figure 5-12 Heated Room Coupled Calculation, Using Dirichlet Temperature Boundary Condition, Response Compared To Measured Thermocouple B-745 Temperatures
Figure 5-13 Heated Room Coupled Calculation, Using Dirichlet Temperature Boundary Condition, Response Compared To Measured Thermocouple B-744 Temperatures

Figure 5-14 Coupled Calculation Heated Room Closure, Using Dirichlet Temperature Boundary, Response Compared To Measured Extensometer Data
5.4. Summary of heated room coupled calculations

Modeling of the WIPP Room B thermal-structural response is challenging even using coupled analysis codes. The coupled analysis effort demonstrated (i.e., a verification) that enclosure radiation methods and Dirichlet temperature conditions can be used effectively. The coupled analysis effort, apart from the one using only conduction and an “equivalent thermal material” in the room (calculation shown in section 5.1), has not validated a “WIPP Room B model” that is as robust as the historic uncoupled thermal-structural method. However, it is believed that incorporation of convection along with radiation may permit this for the case of Room B. The enclosure radiation methods may prove more beneficial when considering high-level waste and/or spent nuclear fuel heat sources in future nuclear waste management storage predictions, as radiative heat transfer may be a significantly more dominant mechanism than convection in those cases.

To summarize the heated room numerical response compared with both the measured vertical closure and horizontal closure data (i.e., experimental data), Figure 5-15 and Figure 5-16 show the Room B vertical and horizontal closure response comparison plot histories. In these images, the measured closure response is compared to uncoupled numerical calculations (using Aria/Adagio with the equivalent thermal material [ETM] model), and three coupled numerical calculations (using Arpeggio with the ETM model, using Arpeggio and Enclosure Radiation [ER] method, and using Arpeggio with the Dirichlet Temperature [DT] boundary condition method). As seen in Figure 5-15, the vertical closure numerical responses, except the Arpeggio ER model, are reasonably predictive, up to approximately 650 days. Thereafter the measured Room B roof response experiences accelerated deformation due to damage and eventual roof separation. Neither of these two phenomena can be captured with the current MD model formulation. This points to a capability gap in the MD Creep constitutive model that will need to be addressed in the future if it is expected to be capable of allowing a numerical model of the room to predict damage and roof separation in a (nuclear waste) repository setting.
Figure 5-15 Numerical Predictions Of Heated Room Vertical Closure Compared To Measured Extensometer Data

Figure 5-16 Numerical Predictions of Heated Room Horizontal Closure Compared To Measured Extensometer Data
As mentioned earlier, a robust air circulation model is one possible strategy to increase fidelity and predictive capability of nuclear waste repository type problems and numerical simulations. This research area is currently being investigated by the SIERRA Mechanics (i.e., Aria) development team.
6. SUMMARY AND CONCLUSIONS

This report has documented currently available code capabilities from SIERRA Mechanics to replicate two historical validation calculations completed in the late 1980 to early 1990 timeframe for the WIPP project. Successful replication of the two historical calculations provides confidence in the use of SIERRA Mechanics for salt waste repository applications and provides a preliminary validation of the isothermal and thermal-mechanical capabilities of the toolset. SIERRA Mechanics was the toolset recommended in the earlier Waste IPSC gap analysis report (Wang, et al., 2011). These two historical validation calculations involved the isothermal WIPP Room D and the heated WIPP Room B in-situ experiments. Both of these test rooms were identical in size and were located at the same stratigraphic horizon. They were also in the same vicinity to each other underground, with the only difference being that one was subjected to a significant thermal load (via heaters in the floor) and the other was not. Measurements of room (tunnel) closure were available for the first few years (1500 days) of Room D’s existence after excavation. Both early-time temperature and room closure measurements were also available for Room B (~1400 days of closure data after excavation and ~1000 days of temperature data after the heaters were activated). These numerical calculations using the SIERRA Mechanics documented in Section 3-5 demonstrate that the new toolset can successfully replicate earlier calculations reasonably well, thus providing a preliminary validation of its thermal-mechanical capabilities.

While the analyses documented herein demonstrate that results from SIERRA Mechanics with the MD model can successfully compare to early-time data from the two in-situ tests at WIPP, the MD model is incapable of capturing fracture and failure processes. So later-time comparisons may suffer. This can be seen in the vertical closure prediction of the Room B calculation. The MD's model successor, the Multi-mechanism Deformation Creep Fracture (MDCF) model (A constitutive model for inelastic flow and damage evolution in solids under triaxial compression, 1992), (Damage-induced nonassociated inelastic flow in rock salt, 1994), (Chan, et al., 1996) has made some initial inroads towards providing this additional capability, but development on the model stopped at Sandia in the mid-1990’s. RESPEC, the company under contract to Sandia at the time of the historical calculations, has continued its attempts to improve the MDCF model for gas cavern applications and has succeeded in correcting certain deficiencies that were identified in the model (DeVries, et al., 2002). However, further improvements of the MDCF model are likely necessary for future salt waste repository applications. Among these, for example, are improvements in the area of healing of the salt upon re-loading of induced fractures and improvements that could incorporate potential moisture effects on salt mechanical response. This is particularly true if, for example, detailed assessments of the evolution of fractures introduced into the salt and the subsequent healing of damage in the “excavation disturbed zone” (EDZ), or alternatively and also known as the "disturbed rock zone" (DRZ), are needed in a future regulatory environment. The initial introduction of damage in the EDZ occurs during construction and may need to characterized more substantially in the salt surrounding panel and/or shaft seals in the future.

Because it was recognized that the MDCF has not been under active development, at least at Sandia, for some time and that it was somewhat dated, it is not currently implemented in SIERRA Mechanics. It also lacks some additional features that recognized leaders in the field of rock salt constitutive modeling are currently including in their state-of-the-art (SOA) rock salt creep models (Benchmarking of geomechanical constitutive models for rock salt (ARMA-10-
Consequently, the MDCF model needs to be further developed so that it incorporates most, if not all, of the advanced features found in other SOA models and incorporated into the SIERRA Mechanics toolset. Additionally, a limited number of these other SOA models (The composite dilatancy model: A constitutive model for the mechanical behavior of rock salt, 2007), (A model for rock salt, describing transient, stationary, and accelerated creep and dilatancy, 2007) from some of the recognized leaders in the field, if available, should be incorporated into the SIERRA Mechanics toolset to allow flexibility in modeling rock salt creeping behavior and permit cross-comparisons with those other models.
7. REFERENCES


APPENDIX A: ISOTHERMAL ROOM CALCULATION INPUT DECK

begin sierra  WIPP Isothermal Room D

title Adagio Simulation of WIPP Room D Closure - MD Model

define direction y with vector 0.0 1.0 0.0
define direction x with vector 1.0 0.0 0.0
define direction z with vector 0.0 0.0 1.0
define direction negative_y with vector 0.0 -1.0 0.0
define point origin with coordinates 0.0 0.0 0.0

#---------- Functions ---------

begin definition for function function_1
    type is piecewise linear
    begin values
        0.  1.0
        3.1536e11  1.0
    end values
end definition for function function_1

begin definition for function function_constant
    type is piecewise linear
    begin values
        0.0               1.0
        1.0e12            1.0
    end values
end definition for function function_constant

#---------- Materials ----------

begin property specification for material CleanSalt
density = 2300.0
begin parameters for model md_creep
    poissons ratio = 0.25
    shear modulus  = 12.4e9
    a1             = 8.386e22
    n1             = 5.5
    q1/r            = 41.96  # 300 K accounted for here
    a2             = 9.672e12
    n2             = 5.0
    q2/r            = 16.79  # 300 K accounted for here
    b1             = 6.086e6
    b2             = 3.034e-2
    qlc            = 5335.0
    sig0           = 20570000.0
    k0             = 6.275e5
    m              = 3.0
    c              = 2.759  # 300 K accounted for here
    alpha          = -17.37
    beta           = -7.738
    deltalc        = 0.58
    amult          = 0.50
    angle          = 0.1
    epstol         = 0.005
    grwfac         = 1.05
    shkfac         = 0.5
    shkfac         = 1.0
    itype          = 0.0
end parameters for model md_creep
end property specification for material CleanSalt
begin property specification for material ArgillaceousSalt
density = 2300.0
begin parameters for model md_creep
  poissons ratio = 0.25
  shear modulus = 12.4e9
  a1 = 1.407e23
  n1 = 5.5
  q1/r = 41.96 # 300 K accounted for here
  a2 = 1.314e13
  n2 = 5.0
  q2/r = 16.79 # 300 K accounted for here
  b1 = 8.998e6
  b2 = 4.289e-2
  qlc = 5335.0
  sig0 = 20570000.0
  k0 = 2.470e6
  m = 3.0
  c = 2.759 # 300 K accounted for here
  alpha = -14.96
  beta = -7.738
  deltalc = 0.58
  amult = 0.50
  angle = 0.1
  epstol = 0.005
  grwfac = 1.05
  # shkfac = 0.5
  shkfac = 1.0
  itype = 0.0
end parameters for model md_creep
end property specification for material ArgillaceousSalt

begin solid section solid_1
  strain incrementation = midpoint_increment
  hourglass rotation = scaled
end solid section solid_1

#---------- Finite Element Model -----------
begin finite element model room
  Database name = roomd.g
  Database type = exodusII

begin parameters for block block_1   #Polyhalite
  material CleanSalt
  material ArgillaceousSalt
  solid mechanics use model md_creep
  section = solid_1
  hourglass stiffness = 0.003
end parameters for block block_1

begin parameters for block block_2  #Argillaceous Halite
  material ArgillaceousSalt
  solid mechanics use model md_creep
  section = solid_1
  hourglass stiffness = 0.003
end parameters for block block_2

begin parameters for block block_3  #Anhydrite
  material CleanSalt
  material ArgillaceousSalt
  solid mechanics use model md_creep
  section = solid_1
  hourglass stiffness = 0.003
end parameters for block block_3
end parameters for block block_3

begin parameters for block block_4  #Halite
  material CleanSalt
  solid mechanics use model md_creep
  section = solid_1
  hourglass stiffness = 0.003
end parameters for block block_4

end finite element model room

begin adagio procedure The_Procedure

#---------- Time Step Control ----------
begin time control
  begin time stepping block p0
    start time = 0.0
    begin parameters for adagio region AdagioRegion
      time increment = 1e-6
    end parameters for adagio region AdagioRegion
  end time stepping block p0
  termination time = 9.504e7
end time control

begin adagio region AdagioRegion
  use finite element model room

  begin adaptive time stepping time
    method = material
    cutback factor = 0.5
    cutback factor = 1.0
    growth factor = 1.05

    maximum multiplier = 1e14
    minimum multiplier = 1.e-4
    maximum failure cutbacks = 10
  end adaptive time stepping time

#---------- Boundary Conditions ----------
begin gravity
  include all blocks
  gravitational constant = 9.79
  direction = negative_y
  function = function_constant
end gravity

begin pressure
  surface = surface_2001  #Top of Model
  function = function_1
  scale factor = 13.57E+06
end pressure

begin pressure
  surface = surface_2000  #Bottom of Model
  function = function_1
  scale factor = 15.97E+06
end pressure

begin fixed displacement
  node set = node_list_100
components = x
end fixed displacement

begin fixed displacement
    node set = nodelist_101
    components = x y
end fixed displacement

begin fixed displacement
    node set = nodelist_102
    components = x
end fixed displacement

begin fixed displacement
    node set = nodelist_400
    components = z
end fixed displacement

begin fixed displacement
    node set = nodelist_401
    components = z
end fixed displacement

#--------- CONTACT MODEL --------------

begin contact definition frictionless
enforcement = frictional
contact surface surf_3000 contains surface_3000
contact surface surf_3001 contains surface_3001
contact surface surf_3002 contains surface_3002
contact surface surf_3003 contains surface_3003
contact surface surf_3004 contains surface_3004
contact surface surf_3005 contains surface_3005
contact surface surf_3006 contains surface_3006
contact surface surf_3007 contains surface_3007
contact surface surf_3008 contains surface_3008
contact surface surf_3009 contains surface_3009
contact surface surf_3010 contains surface_3010
contact surface surf_3011 contains surface_3011
contact surface surf_3012 contains surface_3012
contact surface surf_3013 contains surface_3013
contact surface surf_3014 contains surface_3014
contact surface surf_3015 contains surface_3015
contact surface surf_3016 contains surface_3016
contact surface surf_3017 contains surface_3017

begin interaction Clay_D
    master = surf_3000
    slave = surf_3001
    normal tolerance = 1e-02
    tangential tolerance = 1e-01
    capture tolerance = 1e-02
    tension release = 1.e20
    friction coefficient = 0.2
end interaction Clay_D

begin interaction Clay_E
    master = surf_3002
    slave = surf_3003
    normal tolerance = 1e-02
    tangential tolerance = 1e-01
    capture tolerance = 1e-02
tension release = 1.e20
friction coefficient = 0.2
end interaction Clay_E

begin interaction Clay_F
master = surf_3004
slave = surf_3005
normal tolerance = 1e-02
tangential tolerance = 1e-01
capture tolerance = 1e-02
tension release = 1.e20
friction coefficient = 0.2
end interaction Clay_F

begin interaction Clay_G
master = surf_3006
slave = surf_3007
normal tolerance = 1e-02
tangential tolerance = 1e-01
capture tolerance = 1e-02
tension release = 1.e20
friction coefficient = 0.2
end interaction Clay_G

begin interaction Clay_H
master = surf_3008
slave = surf_3009
normal tolerance = 1e-02
tangential tolerance = 1e-01
capture tolerance = 1e-02
tension release = 1.e20
friction coefficient = 0.2
end interaction Clay_H

begin interaction Clay_I
master = surf_3010
slave = surf_3011
normal tolerance = 1e-02
tangential tolerance = 1e-01
capture tolerance = 1e-02
tension release = 1.e20
friction coefficient = 0.2
end interaction Clay_I

begin interaction Clay_J
master = surf_3012
slave = surf_3013
normal tolerance = 1e-02
tangential tolerance = 1e-01
capture tolerance = 1e-02
tension release = 1.e20
friction coefficient = 0.2
end interaction Clay_J

begin interaction Clay_K
master = surf_3014
slave = surf_3015
normal tolerance = 1e-02
tangential tolerance = 1e-01
capture tolerance = 1e-02
tension release = 1.e20
friction coefficient = 0.2
end interaction Clay_K
begin interaction Clay_L
master = surf_3016
slave = surf_3017
normal tolerance = 1e-02
tangential tolerance = 1e-01
capture tolerance = 1e-02
tension release = 1.e20
friction coefficient = 0.2
end interaction Clay_L

design contact definition frictionless

#--------- Initial Conditions ---------
begin initial condition
include all blocks
# initialize variable name = unrotated_stress
initialize variable name = stress
variable type = element
subroutine real parameter: top = 52.87
subroutine real parameter: bot = -54.19
subroutine real parameter: p1 = -13.57e6
subroutine real parameter: po = -15.97e6
subroutine real parameter: kvert_xx = 1.0
subroutine real parameter: kvert_yy = 1.0
subroutine real parameter: kvert_zz = 1.0
subroutine real parameter: kvert_xy = 0.0
subroutine real parameter: kvert_yz = 0.0
subroutine real parameter: kvert_zx = 0.0
subroutine string parameter: dir = Y
element block subroutine = geo_is
end initial condition

#--------- Results Output ---------
begin results output output_1
database name = roomd.e
database type = exodusII
at time 0.0 increment = 1.0e-6
at time 1.0e-6 increment = 432000.0
# at time 31536000.0 increment = 31536000.0
nodal variables = displacement as displ
nodal variables = residual as resid
element variables = unrotated_stress as sig
element variables = stress
element variables = log_strain as strain
element variables = von_mises as vommis
element variables = eqcs as eqcs
element variables = nsub, zeta, capf, lode
global variables = total_iter as itotal
end results output output_1

#--------- Solver ---------
Begin solver
begin loadstep predictor
type = scale_factor
scale factor = 1.0
end loadstep predictor

begin control contact
level = 1
  target relative residual = 0.005
  acceptable relative residual = 100.0
  maximum iterations = 100
end control contact

begin cg
  target relative residual = 0.0005
  acceptable relative residual = 0.01
  maximum iterations = 3000
  iteration print = 100
  line search tangent
  preconditioner = diagonal
end cg

end solver

end adagio region AdagioRegion

end adagio procedure The_Procedure

end sierra WIPP Isothermal Room D
APPENDIX B: HEATED ROOM UNCOUPLED CALCULATION INPUT DECKS

# directory : /scratch/jsrath/NEAMS/roomb/thermal/simu301
# file : aria.i
# author : Jonathan Scott Rath
# description : NEAMS Room B Aria input deck
# Model 2 (Room B, Thermal)
# revision_log : 29/AUGUST/2011
# - Adapted heat flux at Room B opening to account
#   for normal outward direction
# : 20/JUNE/2011
# - Added convection heat transfer boundary condition
#   (Side Set 4000, h=0.51 W/m^2/K)
# : 06/MAY/2011
# - Added 3dHex8 MESH & 3dHex27 MESH variable control
# - Added non-conditional function tpf.include
# - Added non-conditional function ntc.include
# - Added coefficient of thermal expansion
# - Added power law thermal conductivity form
# : 03/MAY/2011
# - First Edition
# unit system : System International (SI)
# - mass = gram (kg)
# - length = meter (m)
# - time = seconds (sec)
# - Temperature = Kelvin
# - density = kg/(m^3)
# - velocity = meter/sec = 10^-3*km/sec
# - acceleration = m/(sec^2)
# - force = mass * acceleration = kg*m/sec^2
# - pressure = Newton / (m^2)
# - energy = Newton*m
# - power = Joule/sec
# - = Newton*m/sec
# - = Watt
# BEGIN SIERRA roomb_thermal

title NEAMS Room B thermal response simulation using Aria
restart = automatic

define direction y with vector 0.0 1.0 0.0
define direction x with vector 1.0 0.0 0.0
define direction z with vector 0.0 0.0 1.0

define point origin with coordinates 0.0 0.0 0.0

### Function definitions

Begin definition for function thermal_power_flux
Abscissa = time # [second]
Ordinate = thermal_power_flux # [watt (Nm/s)]/(meter^2)
Type = analytic
Evaluate Expression = "x <= 2808000 ? 0.0 : 228.012039*exp(-7.327e-10*x);"
Differentiate Expression is "x <= 2808000 ? 0.0 : -1.67064421e-07*exp(-7.327e-10*x);"
End definition for function thermal_power_flux

### Define materials for Aria region
###

Begin Aria material ONE
    density = constant rho = 2300 # [kg/m^3]
    thermal conductivity = power_law a = 3333.406168 gamma = -1.14
    specific heat = constant cp = 860 # [joule (Nm)]/(kilogram*degK)
    heat conduction = basic
End Aria material ONE

Begin Aria material TWO
    density = constant rho = 1 # [kg/m^3]
    thermal conductivity = constant k = 50 # [watt (Nm/s)]/(meter*degK)
    specific heat = constant cp = 1000 # [joule (Nm)]/(kilogram*degK)
    heat conduction = basic
End Aria material TWO

### Aria Finite Element Model
###

Begin finite element model Aria_FEM
    Database Name = roombq.g
    Use material ONE for block_1
    Use material TWO for block_2
    Coordinate system is cartesian
End finite element model Aria_FEM

### Define Aria solver parameters
###

Begin aztec equation solver AriaSystemEquationSolver
    Solution Method = cg
    Preconditioning Method = DD-ICC
    Maximum Iterations = 500
    Residual Norm Tolerance = 1e-08
    Residual Norm Scaling = r0
End aztec equation solver AriaSystemEquationSolver

### Define global constants
###

Begin Global Constants
    Stefan Boltzmann Constant = 5.67e-08 # [watt (Nm/s)]/(meter^2*degK^4)
End

### Define Output Error File
###

Begin Postprocessor Output Control pp_out
    Comment Character Is %
    Write To File Errors_roombq.dat
    Floating Point Precision Is 8
Floating Point Format Is Scientific
End Postprocessor Output Control pp_out

### Define Solution procedure

Begin procedure AriaProcedure

Begin Solution Control Description
  Use System Main
  Begin System Main
    Begin Transient Time_Block_1
      Advance AriaRegion
    End
    Begin Transient Time_Block_2
      Advance AriaRegion
    End
  End

Begin Parameters For Transient Time_Block_1
  Start Time = 0
  Termination Time = 17280000
  Begin Parameters For Aria Region AriaRegion
    Time Integration Method = Second_Order
    Time Step Variation = Adaptive
    Initial Time step Size = 100
    Minimum Time step Size = 50
    Maximum Time step Size = 864000
    Maximum Time Step Size ratio = 10
    Minimum Resolved Time Step Size = 50
    Predictor-Corrector Tolerance = 0.0005
    Predictor-Corrector Normalization = MAX
  End

Begin Parameters For Transient Time_Block_2
  Start Time = 17280000
  Termination Time = 157784630.4
  Begin Parameters For Aria Region AriaRegion
    Time Integration Method = Second_Order
    Time Step Variation = Adaptive
    Initial Time step Size = 100
    Minimum Time step Size = 50
    Maximum Time step Size = 864000
    Maximum Time Step Size ratio = 10
    Minimum Resolved Time Step Size = 50
    Predictor-Corrector Tolerance = 0.0005
    Predictor-Corrector Normalization = MAX
  End
End

End Solution Control Description

### Define Aria Region

Begin Aria Region AriaRegion

  Use finite element model Aria_FEM
  Use linear solver AriaSystemEquationSolver

  nonlinear solution strategy = Newton
NONLINEAR RESIDUAL TOLERANCE = 1.0e-6
MAXIMUM NONLINEAR ITERATIONS = 5
NONLINEAR RELAXATION FACTOR = 1.0

use dof averaged nonlinear residual

accept solution after maximum nonlinear iterations = true

EQ Energy for Temperature on block_1 using Q1 with Lumped_Mass DIFF #SRC
EQ Energy for Temperature on block_2 using Q1 with Lumped_Mass DIFF #SRC

### Initial Conditions

IC const on all_blocks Temperature = 300

### Boundary Conditions

# Adiabatic or Isentropic BC (i.e., "von Neuman") energy flux = 0
# von Neuman B.C. left symmetry
BC Flux for Energy on surface_1000 = constant flux = 0.0
# von Neuman B.C. right far-field
BC Flux for Energy on surface_1001 = constant flux = 0.0
# von Neuman B.C. y-vertical bottom model
BC Flux for Energy on surface_2000 = constant flux = 0.0
# von Neuman B.C. y-vertical top model
BC Flux for Energy on surface_2001 = constant flux = 0.0

# Convective heat transfer, q = H * (T-T_REF)
# Heat Flux due to natural heat convection (WIPP room heat loss)
BC Flux for Energy on surface_4000 = Nat_Conv T_REF = 300 H = 0.18

### Heat Source

# BC Flux for Energy on surface_6666 = Function Name = thermal_power_flux

Begin Heat Flux Boundary Condition DHLW
Add Surface surface_6666
Flux Time Function = thermal_power_flux
End Heat Flux Boundary Condition DHLW

### Post Processing

PostProcess HEAT_FLUX on All_Blocks using Q1

### Output Aria results
Begin Results Output output
Database Name = roombq.e
Database Type = ExodusII
Global Variables = time_step as timestep
Nodal Variables = solution->temperature as temp
Nodal Variables = pp->heat_flux as heatflux
Timestep Adjustment Interval = 4
At time 0, Increment = 604800 # ( t=0 seconds, incr=1 weeks )
At time 15778463.04, Increment = 2629743.84 # ( t=0.5 years, incr=1 months )
At time 31556926.08, Increment = 2629743.84 # ( t=1 years, incr=1 months )
At time 63113852.16, Increment = 2629743.84 # ( t=2 years, incr=1 months )
At time 94670778.24, Increment = 2629743.84 # ( t=3 years, incr=1 months )
At time 126227704.3, Increment = 2629743.84 # ( t=4 years, incr=1 months )
At time 157784630.4, Increment = 2629743.84 # ( t=5 years, incr=1 months )
Termination Time = 157784630.4 # 5 years
End Results Output output

Begin History Output history_output
Database Name = roombq.h
Database Type = ExodusII
At time 0, Increment = 604800 # ( t=0 seconds, incr=1 weeks )
At time 15778463.04, Increment = 2629743.84 # ( t=0.5 years, incr=1 months )
At time 31556926.08, Increment = 2629743.84 # ( t=1 years, incr=1 months )
At time 63113852.16, Increment = 2629743.84 # ( t=2 years, incr=1 months )
At time 94670778.24, Increment = 2629743.84 # ( t=3 years, incr=1 months )
At time 126227704.3, Increment = 2629743.84 # ( t=4 years, incr=1 months )
At time 157784630.4, Increment = 2629743.84 # ( t=5 years, incr=1 months )
Termination Time = 157784630.4 # 5 years
Node solution->temperature Nearest Location 0.0 -1.08 -0.762 as A1
Node solution->temperature Nearest Location 0.0 -1.54 -0.762 as A2
Node solution->temperature Nearest Location 0.0 -1.99 -0.762 as A3
Node solution->temperature Nearest Location 0.0 -2.38 -0.762 as A4
Node solution->temperature Nearest Location 0.0 -2.91 -0.762 as A5
Node solution->temperature Nearest Location 0.0 -3.29 -0.762 as A6
Node solution->temperature Nearest Location 0.0 -4.20 -0.762 as A7
Node solution->temperature Nearest Location 0.0 -5.12 -0.762 as A8
Node solution->temperature Nearest Location 0.0 -5.96 -0.762 as A9
Node solution->temperature Nearest Location 0.0 -6.03 -0.762 as A10
Node solution->temperature Nearest Location 0.0 -6.95 -0.762 as A11
Node solution->temperature Nearest Location 0.0 -10.22 -0.762 as A12
Node solution->temperature Nearest Location 0.0 -16.32 -0.762 as A13
Node solution->temperature Nearest Location 0.15 -1.08 -0.762 as B1
Node solution->temperature Nearest Location 0.15 -3.37 -0.762 as B2
Node solution->temperature Nearest Location 0.15 -4.01 -0.762 as B3
Node solution->temperature Nearest Location 0.15 -4.65 -0.762 as B4
Node solution->temperature Nearest Location 0.15 -5.32 -0.762 as B5
Node solution->temperature Nearest Location 0.15 -5.96 -0.762 as B6
Node solution->temperature Nearest Location 0.21 -1.08 -0.762 as C1
Node solution->temperature Nearest Location 0.21 -2.38 -0.762 as C2
Node solution->temperature Nearest Location 0.21 -3.29 -0.762 as C3
Node solution->temperature Nearest Location 0.21 -4.20 -0.762 as C4
Node solution->temperature Nearest Location 0.21 -5.12 -0.762 as C5
Node solution->temperature Nearest Location 0.21 -6.03 -0.762 as C6
Node solution->temperature Nearest Location 0.21 -6.95 -0.762 as C7
Node solution->temperature Nearest Location 0.40 -1.08 -0.762 as D1
Node solution->temperature Nearest Location 0.40 -2.38 -0.762 as D2
Node solution->temperature Nearest Location 0.40 -3.29 -0.762 as D3
Node solution->temperature Nearest Location 0.40 -4.20 -0.762 as D4
Node solution->temperature Nearest Location 0.40 -5.12 -0.762 as D5
Node solution->temperature Nearest Location 0.40 -6.03 -0.762 as D6
Node solution->temperature Nearest Location 0.40 -6.95 -0.762 as D7
Node solution->temperature Nearest Location 0.76 -1.08 -0.762 as E1

85
<table>
<thead>
<tr>
<th>Node solution-&gt;temperature</th>
<th>Nearest Location</th>
<th>0.76</th>
<th>-2.38</th>
<th>-0.762  as E2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.76</td>
<td>-3.29</td>
<td>-0.762  as E3</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.76</td>
<td>-4.20</td>
<td>-0.762  as E4</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.76</td>
<td>-5.12</td>
<td>-0.762  as E5</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.76</td>
<td>-6.03</td>
<td>-0.762  as E6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.76</td>
<td>-6.95</td>
<td>-0.762  as E7</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>1.13</td>
<td>-1.08</td>
<td>-0.762  as F1</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>1.31</td>
<td>-1.51</td>
<td>-0.762  as F2</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>1.49</td>
<td>-1.93</td>
<td>-0.762  as F3</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>1.83</td>
<td>-2.76</td>
<td>-0.762  as F4</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.01</td>
<td>-1.08</td>
<td>-0.762  as F5</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>4.63</td>
<td>-9.52</td>
<td>-0.762  as F6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>6.98</td>
<td>-15.16</td>
<td>-0.762  as F7</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>2.75</td>
<td>-1.08</td>
<td>-0.762  as G1</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.09</td>
<td>-1.42</td>
<td>-0.762  as G2</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.39</td>
<td>-1.72</td>
<td>-0.762  as G3</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>4.03</td>
<td>-2.36</td>
<td>-0.762  as G4</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>6.19</td>
<td>-4.52</td>
<td>-0.762  as G5</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>9.21</td>
<td>-7.54</td>
<td>-0.762  as G6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>13.54</td>
<td>-11.87</td>
<td>-0.762  as G7</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>2.75</td>
<td>-0.62</td>
<td>-0.762  as H1</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.21</td>
<td>-0.62</td>
<td>-0.762  as H2</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.66</td>
<td>-0.62</td>
<td>-0.762  as H3</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>4.58</td>
<td>-0.62</td>
<td>-0.762  as H4</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>7.63</td>
<td>-0.62</td>
<td>-0.762  as H5</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>11.89</td>
<td>-0.62</td>
<td>-0.762  as H6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>17.99</td>
<td>-0.62</td>
<td>-0.762  as H7</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>2.75</td>
<td>1.67</td>
<td>-0.762  as I1</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.21</td>
<td>1.67</td>
<td>-0.762  as I2</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.66</td>
<td>1.67</td>
<td>-0.762  as I3</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>4.58</td>
<td>1.67</td>
<td>-0.762  as I4</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>7.63</td>
<td>1.67</td>
<td>-0.762  as I5</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>11.89</td>
<td>1.67</td>
<td>-0.762  as I6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>17.99</td>
<td>1.67</td>
<td>-0.762  as I7</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>2.75</td>
<td>3.96</td>
<td>-0.762  as J1</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.21</td>
<td>3.96</td>
<td>-0.762  as J2</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.66</td>
<td>3.96</td>
<td>-0.762  as J3</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>4.58</td>
<td>3.96</td>
<td>-0.762  as J4</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>7.63</td>
<td>3.96</td>
<td>-0.762  as J5</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>11.89</td>
<td>3.96</td>
<td>-0.762  as J6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>17.99</td>
<td>3.96</td>
<td>-0.762  as J7</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>2.75</td>
<td>4.42</td>
<td>-0.762  as K1</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.09</td>
<td>4.76</td>
<td>-0.762  as K2</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>3.39</td>
<td>5.06</td>
<td>-0.762  as K3</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>4.03</td>
<td>5.70</td>
<td>-0.762  as K4</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>6.19</td>
<td>7.86</td>
<td>-0.762  as K5</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>9.21</td>
<td>10.88</td>
<td>-0.762  as K6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>13.54</td>
<td>15.21</td>
<td>-0.762  as K7</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>4.42</td>
<td>-0.762  as L1</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>4.88</td>
<td>-0.762  as L2</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>5.33</td>
<td>-0.762  as L3</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>6.25</td>
<td>-0.762  as L4</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>9.30</td>
<td>-0.762  as L5</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>13.56</td>
<td>-0.762  as L6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>15.21</td>
<td>-0.762  as L7</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>5.02</td>
<td>-0.762  as AB6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>5.32</td>
<td>-0.762  as AB5</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>6.22</td>
<td>-0.762  as AB4</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>9.32</td>
<td>-0.762  as AB3</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>13.62</td>
<td>-0.762  as AB2</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>19.72</td>
<td>-0.762  as AB1</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>-1.68</td>
<td>-0.762  as BE6</td>
</tr>
<tr>
<td>Node solution-&gt;temperature</td>
<td>Nearest Location</td>
<td>0.00</td>
<td>-1.98</td>
<td>-0.762  as BE5</td>
</tr>
</tbody>
</table>
Node solution->temperature Nearest Location  0.00  -2.88  -0.762  as BE4
Node solution->temperature Nearest Location  0.00  -5.98  -0.762  as BE3
Node solution->temperature Nearest Location  0.00  -10.28  -0.762  as BE2
Node solution->temperature Nearest Location  0.00  -16.38  -0.762  as BE1

End History Output history_output

End Aria Region AriaRegion

End procedure AriaProcedure

END SIERRA roomb_thermal
BEGIN SIERRA roomb_structural

Begin diagnostic control Adagio_Diagnostics
  enable "tangent"
End diagnostic control Adagio_Diagnostics

title NEAMS Room B structural response simulation using Adagio

define direction x with vector 1.0 0.0 0.0
define direction y with vector 0.0 1.0 0.0
define direction z with vector 0.0 0.0 1.0

define point origin with coordinates 0.0 0.0 0.0

###
### Function definitions
###

Begin definition for function gravitational_acceleration_function
  Type is piecewise linear
  Begin values
    0 1
    157784630.4 1
  End values
End definition for function gravitational_acceleration_function

Begin definition for function lithostatic_pressure_ybot_function
  Type is piecewise linear
  Begin values
    0 15980670.02
    157784630.4 15980670.02
  End values
End definition for function lithostatic_pressure_ybot_function

Begin definition for function lithostatic_pressure_ytop_function
  Type is piecewise linear
  Begin values
    0
  End values
End definition for function lithostatic_pressure_ytop_function
Begin values
    0  13570000
    157784630.4  13570000
End values
End definition for function lithostatic_pressure_ytop_function

#   T_max = 1500 [Kelvin]
#   T_ref = 300 [Kelvin]
#   alpha = 2.4e-05 [1/Kelvin]
#   ----------------------------
#   T_ref    0.0
#   T_max    (T_max-T_ref)*alpha
#   ----------------------------

Begin definition for function polyhalite_thermal_strain_function
Type is piecewise linear
Begin values
    300 0
    1500 0.0288
End values
End definition for function polyhalite_thermal_strain_function

#   alpha = 4e-05 [1/Kelvin]
#   ----------------------------
#   T_ref    0.0
#   T_max    (T_max-T_ref)*alpha
#   ----------------------------

Begin definition for function argillaceous_thermal_strain_function
Type is piecewise linear
Begin values
    300 0
    1500 0.048
End values
End definition for function argillaceous_thermal_strain_function

#   alpha = 2e-05 [1/Kelvin]
#   ----------------------------
#   T_ref    0.0
#   T_max    (T_max-T_ref)*alpha
#   ----------------------------

Begin definition for function anhydrite_thermal_strain_function
Type is piecewise linear
Begin values
    300 0
    1500 0.024
End values
End definition for function anhydrite_thermal_strain_function

#   alpha = 4.5e-05 [1/Kelvin]
#   ----------------------------
#   T_ref    0.0
#   T_max    (T_max-T_ref)*alpha
#   ----------------------------

Begin definition for function halite_thermal_strain_function
Type is piecewise linear
Begin values
    300 0
    1500 0.054
End values
End definition for function halite_thermal_strain_function

Begin definition for function polyhalite_pressure_volstrain_function
Type is piecewise linear
Ordinate is volumetric_strain
Abscissa is Pressure
Begin values
-1  -6.583333333e+10 # -65833.33333 MPa
  0  0
  1  6.583333333e+10 # 65833.33333 MPa
End values
End definition for function polyhalite_pressure_volstrain_function

Begin definition for function anhydrite_pressure_volstrain_function
  Type is piecewise linear
  Ordinate is volumetric_strain
  Abscissa is Pressure
Begin values
-1  -8.344444444e+10 # -83444.44444 MPa
  0  0
  1  8.344444444e+10 # 83444.44444 MPa
End values
End definition for function anhydrite_pressure_volstrain_function

### Element Sections
###

Begin solid section hex8
  Strain Incrementation = midpoint_increment
  Hourglass rotation = scaled
End solid section hex8
###

### Material Models
###

Begin property specification for material polyhalite
  Density = 2300
  thermal strain x function = polyhalite_thermal_strain_function
  thermal strain y function = polyhalite_thermal_strain_function
  thermal strain z function = polyhalite_thermal_strain_function
Begin parameters for model soil_foam
  youngs modulus = 5.53e+10 # [Pa]
  poissons ratio = 0.36 # [dimensionless]
  bulk modulus = 6.583333333e+10 # [Pa]
  shear modulus = 2.033088235e+10 # [Pa]
  a0 = 2459512.147 # [Pa]
  a1 = 2.457780096
  a2 = 0 # [1/Pa]
  pressure cutoff = -1000704.722 # [Pa]
  pressure function = polyhalite_pressure_volstrain_function
End parameters for model soil_foam
End property specification for material polyhalite

Begin property specification for material argillaceous
  Density = 2300
  thermal strain x function = argillaceous_thermal_strain_function
  thermal strain y function = argillaceous_thermal_strain_function
  thermal strain z function = argillaceous_thermal_strain_function
Begin Parameters For Model MD_Creep
  # Youngs Modulus = 3.100000833e+10
  # Poissons Ratio = 0.250000336
  # Lambda = 1.240003333e+10
  # Two Mu = 2.48e+10
  Bulk Modulus = 2.06667e+10
  Shear Modulus = 1.24e+10
  A1 = 1.406e+23
Q1/R = 12581.78
# Q1/RT = 41.93926667 # Isothermal, T=300 Kelvin
N1 = 5.5
B1 = 8993300
A2 = 1.3131e+13
Q2/R = 5032.71
# Q2/RT = 16.7757 # Isothermal, T=300 Kelvin
N2 = 5
B2 = 0.042875
Sig0 = 20570000
Qlc = 5335
M = 3
K0 = 2470000
#
CSTAR = 0.009189
#
TK = 300
#
C = 2.759 # C = CSTAR/TK (MD Creep model uses C when isothermal)  
C = 0.009189 # C (MD Creep model uses C=CSTAR when nonisothermal)

End Parameters For Model MD_Creep

End property specification for material argillaceous

Begin property specification for material anhydrite
Density = 2300
thermal strain x function = anhydrite_thermal_strain_function
thermal strain y function = anhydrite_thermal_strain_function
thermal strain z function = anhydrite_thermal_strain_function

Begin parameters for model soil_foam
  youngs modulus = 7.51e+10 # [Pa]
  poissons ratio = 0.35 # [dimensionless]
  bulk modulus = 8.344444444e+10 # [Pa]
  shear modulus = 2.781481481e+10 # [Pa]
  a0 = 2338268.59 # [Pa]
  a1 = 2.33826859
  a2 = 0 # [1/Pa]
  pressure cutoff = -1000000 # [Pa]
  pressure function = anhydrite_pressure_volstrain_function

End parameters for model soil_foam

End property specification for material halite
Density = 2300
thermal strain x function = halite_thermal_strain_function
thermal strain y function = halite_thermal_strain_function
thermal strain z function = halite_thermal_strain_function

Begin Parameters For Model MD_Creep
  Youngs Modulus = 3.118558614e+10
  Poissons Ratio = 0.2484221834
  Lambda = 1.233333333e+10
  Two Mu = 2.498e+10
  Bulk Modulus = 2.066e+10
  Shear Modulus = 1.249e+10
  A1 = 8.386e+22
  Q1/R = 12581.78158
# Q1/RT = 41.93927193 # Isothermal, T=300 Kelvin
N1 = 5.5
B1 = 6086000
A2 = 9.672e+12
Q2/RT = 5032.712632
# Q2/RT = 16.77570877 # Isothermal, T=300 Kelvin
N2 = 5
B2 = 0.03034
Sig0 = 20570000
Qlc = 5335
M = 3
K0 = 627500
# CSTAR = 0.009189
# TK = 300
# C = 2.759 # C = CSTAR/TK (MD Creep model uses C when isothermal)
C = 0.009189 # C (MD Creep model uses C=CSTAR when nonisothermal)
Alpha = -17.37
Beta = -7.738
Deltalc = 0.58
Amult = 0.5
Grwfac = 1.05
Epstol = 0.005
Shkfac = 1
Itype = 0
Angle = 0.1
End Parameters For Model MD_Creep
End property specification for material halite
###
### Adagio Finite Element Model
###

Begin finite element model Adagio_FEM

database name = roomb.g
database type = exodusII

begin parameters for block block_1
material polyhalite
solid mechanics use model soil_foam
section = hex8
hourglass stiffness = 0.003
end parameters for block block_1

begin parameters for block block_2
material argillaceous
solid mechanics use model MD_Creep
section = hex8
hourglass stiffness = 0.003
end parameters for block block_2

begin parameters for block block_3
material anhydrite
solid mechanics use model soil_foam
section = hex8
hourglass stiffness = 0.003
end parameters for block block_3

begin parameters for block block_4
material halite
solid mechanics use model MD_Creep
section = hex8
hourglass stiffness = 0.003
end parameters for block block_4

End finite element model Adagio_FEM

###
### Define Solution procedure
###

Begin adagio procedure AdagioProcedure

Begin Time Control

Begin Time Stepping block tsb1
Start Time = 0
Begin parameters for adagio region AdagioRegion
Time Increment = 1e-06
End parameters for adagio region AdagioRegion
End Time Stepping Block tsb1

Termination time = 157784630.4

End Time control

Begin adagio region AdagioRegion

Use finite element model adagio_FEM

###
### Contact Definitions
###

Begin Contact Definition WIPP_Room_B_Clay_Seams

Enforcement = Frictional

Contact Surface surf_3000 contains surface_3000
Contact Surface surf_3001 contains surface_3001
Contact Surface surf_3002 contains surface_3002
Contact Surface surf_3003 contains surface_3003
Contact Surface surf_3004 contains surface_3004
Contact Surface surf_3005 contains surface_3005
Contact Surface surf_3006 contains surface_3006
Contact Surface surf_3007 contains surface_3007
Contact Surface surf_3008 contains surface_3008
Contact Surface surf_3009 contains surface_3009
Contact Surface surf_3010 contains surface_3010
Contact Surface surf_3011 contains surface_3011
Contact Surface surf_3012 contains surface_3012
Contact Surface surf_3013 contains surface_3013
Contact Surface surf_3014 contains surface_3014
Contact Surface surf_3015 contains surface_3015
Contact Surface surf_3016 contains surface_3016
Contact Surface surf_3017 contains surface_3017

Begin Interaction Clay_D
Master = surf_3000
Slave = surf_3001
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_D

Begin Interaction Clay_E
  Master = surf_3002
  Slave = surf_3003
    Normal Tolerance = 0.01
    Tangential Tolerance = 0.1
    Capture Tolerance = 0.01
    Tension Release = 1e+20
    Friction Coefficient = 0.2
End Interaction Clay_E

Begin Interaction Clay_F
  Master = surf_3004
  Slave = surf_3005
    Normal Tolerance = 0.01
    Tangential Tolerance = 0.1
    Capture Tolerance = 0.01
    Tension Release = 1e+20
    Friction Coefficient = 0.2
End Interaction Clay_F

Begin Interaction Clay_G
  Master = surf_3006
  Slave = surf_3007
    Normal Tolerance = 0.01
    Tangential Tolerance = 0.1
    Capture Tolerance = 0.01
    Tension Release = 1e+20
    Friction Coefficient = 0.2
End Interaction Clay_G

Begin Interaction Clay_H
  Master = surf_3008
  Slave = surf_3009
    Normal Tolerance = 0.01
    Tangential Tolerance = 0.1
    Capture Tolerance = 0.01
    Tension Release = 1e+20
    Friction Coefficient = 0.2
End Interaction Clay_H

Begin Interaction Clay_I
  Master = surf_3010
  Slave = surf_3011
    Normal Tolerance = 0.01
    Tangential Tolerance = 0.1
    Capture Tolerance = 0.01
    Tension Release = 1e+20
    Friction Coefficient = 0.2
End Interaction Clay_I

Begin Interaction Clay_J
  Master = surf_3012
  Slave = surf_3013
    Normal Tolerance = 0.01
    Tangential Tolerance = 0.1
    Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_J

Begin Interaction Clay_K
Master = surf_3014
Slave = surf_3015
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_K

Begin Interaction Clay_L
Master = surf_3016
Slave = surf_3017
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_L

End Contact Definition WIPP_Room_B_Clay_Seams

### Database Results Output Definitions

Begin Results Output adagio_output

database name = roomb.e
database type = exodusII

At Time 0 Increment = 600 # Every 10.0 minutes
At Time 3600 Increment = 3600 # Every hour
At Time 86400 Increment = 86400 # Every day
At Time 604800 Increment = 604800 # Every Week
At Time 2629743.84 Increment = 2629743.84 # Every Month
At Time 15778463.04 Increment = 7889231.52 # Every 0.25*year

Global Variables = timestep as timestep
Global Variables = kinetic_energy as ke
Global Variables = contact_energy as ce

Nodal Variables = velocity as vel
Nodal Variables = displacement as displ

Element Variables = stress as sig
Element Variables = unrotated_stress as usig
Element Variables = von_mises as vonmises
Element Variables = hydrostatic_stress as pressure
Element Variables = stress_invariant_1 as sinv1
Element Variables = stress_invariant_2 as sinv2
Element Variables = stress_invariant_3 as sinv3
Element Variables = max_principal_stress as psigm1
Element Variables = intermediate_principal_stress as psigm2
Element Variables = min_principal_stress as psigm3
Element Variables = max_shear_stress
Element Variables = octahedral_shear_stress as octahedral
Element Variables = temperature as temp
Element Variables = log_strain as strain
Element Variables = log_strain_invariant_1 as volstrain

End Results Output adagio_output

### Database History Output Definitions

Begin History Output adagio_history
database name = roomb.h
database type = exodusII
At Time 0 Increment = 600 # Every 10.0 minutes
At Time 3600 Increment = 3600 # Every hour
At Time 86400 Increment = 86400 # Every day
At Time 604800 Increment = 604800 # Every Week
At Time 2629743.84 Increment = 2629743.84 # Every Month
At Time 15778463.04 Increment = 7889231.52 # Every 0.25*year
Node displacement Nearest Location 0.0 -1.08 0 as A1
Node displacement Nearest Location 0.0 -1.54 0 as A2
Node displacement Nearest Location 0.0 -1.99 0 as A3
Node displacement Nearest Location 0.0 -2.38 0 as A4
Node displacement Nearest Location 0.0 -2.91 0 as A5
Node displacement Nearest Location 0.0 -3.29 0 as A6
Node displacement Nearest Location 0.0 -4.20 0 as A7
Node displacement Nearest Location 0.0 -5.12 0 as A8
Node displacement Nearest Location 0.0 -5.96 0 as A9
Node displacement Nearest Location 0.0 -6.03 0 as A10
Node displacement Nearest Location 0.0 -6.95 0 as A11
Node displacement Nearest Location 0.0 -10.22 0 as A12
Node displacement Nearest Location 0.0 -16.32 0 as A13
Node displacement Nearest Location 2.75 -1.08 0 as G1
Node displacement Nearest Location 3.09 -1.42 0 as G2
Node displacement Nearest Location 3.39 -1.72 0 as G3
Node displacement Nearest Location 4.03 -2.36 0 as G4
Node displacement Nearest Location 6.19 -4.52 0 as G5
Node displacement Nearest Location 9.21 -7.54 0 as G6
Node displacement Nearest Location 13.54 -11.87 0 as G7
Node displacement Nearest Location 2.75 1.67 0 as I1
Node displacement Nearest Location 3.21 1.67 0 as I2
Node displacement Nearest Location 3.66 1.67 0 as I3
Node displacement Nearest Location 4.58 1.67 0 as I4
Node displacement Nearest Location 7.63 1.67 0 as I5
Node displacement Nearest Location 11.89 1.67 0 as I6
Node displacement Nearest Location 17.99 1.67 0 as I7
Node displacement Nearest Location 2.75 4.42 0 as K1
Node displacement Nearest Location 3.09 4.76 0 as K2
Node displacement Nearest Location 3.39 5.06 0 as K3
Node displacement Nearest Location 4.03 5.70 0 as K4
Node displacement Nearest Location 6.19 7.86 0 as K5
Node displacement Nearest Location 9.21 10.88 0 as K6
Node displacement Nearest Location 13.54 15.21 0 as K7
Node displacement Nearest Location 0.00 4.42 0 as L1
Node displacement Nearest Location 0.00 4.88 0 as L2
Node displacement Nearest Location 0.00 5.33 0 as L3
Node displacement Nearest Location 0.00 6.25 0 as L4
Node displacement Nearest Location 0.00 9.30 0 as L5
Node displacement Nearest Location 0.00 13.56 0 as L6
Node displacement Nearest Location 0.00 15.21 0 as L7
Node displacement Nearest Location 2.75 0.30 0 as M1
Node displacement Nearest Location 3.66 0.30 0 as M2
Node displacement Nearest Location 4.58 0.30 0 as M3
Node displacement Nearest Location 7.63 0.30 0 as M4
Node displacement Nearest Location 11.89 0.30 0 as M5
Node displacement Nearest Location 17.99 0.30 0 as M6
Node displacement Nearest Location  2.75  -0.78  0  as N1
Node displacement Nearest Location  17.99  -0.78  0  as N2
Node displacement Nearest Location  2.75   4.12  0  as O1
Node displacement Nearest Location  17.99   4.12  0  as O2
Element stress Nearest Location  0.00  -1.08  -0.225  as P1
Element stress Nearest Location  0.00  -4.73  -0.225  as P2
Element stress Nearest Location  0.46  -1.08  -0.225  as Q1
Element stress Nearest Location  0.46  -8.69  -0.225  as Q2
Element stress Nearest Location  0.46  -16.32  -0.225  as Q3
Element stress Nearest Location  2.75   1.21  -0.225  as R1
Element stress Nearest Location  10.36   1.21  -0.225  as R2
Element stress Nearest Location  17.99   1.21  -0.225  as R3
Element stress Nearest Location  2.75   1.67  -0.225  as S1
Element stress Nearest Location  6.40   1.67  -0.225  as S2
Element stress Nearest Location  9.14   1.67  -0.225  as S3
Element stress Nearest Location  13.11   1.67  -0.225  as S4
Element stress Nearest Location  24.08   1.67  -0.225  as S5
Element stress Nearest Location  2.75   2.13  -0.225  as T1
Element stress Nearest Location  10.36   2.13  -0.225  as T2
Element stress Nearest Location  17.99   2.13  -0.225  as T3
Element stress Nearest Location  0.46   4.42  -0.225  as U1
Element stress Nearest Location  0.46  12.03  -0.225  as U2
Element stress Nearest Location  0.46  19.66  -0.225  as U3
Element stress Nearest Location  0.00   4.42  -0.225  as V1
Element stress Nearest Location  0.00   8.07  -0.225  as V2

### Initial Conditions

# Hydrostatic pressure initial condition (varies according to y-direction)
Begin initial condition initialize_stress_state
  Initialize variable name = unrotated_stress
  Variable type = element
  Include All Blocks
  Element Block Subroutine = geo_is
  Subroutine Real Parameter: bot = -54.19
  Subroutine Real Parameter: top = 52.87
  Subroutine Real Parameter: po = -15980670.02
  Subroutine Real Parameter: pl = -13570000
  Subroutine Real Parameter: kvert_xx = 1
  Subroutine Real Parameter: kvert_yy = 1
  Subroutine Real Parameter: kvert_zz = 1
  Subroutine Real Parameter: kvert_xy = 0
  Subroutine Real Parameter: kvert_yz = 0
  Subroutine Real Parameter: kvert_zx = 0
  Subroutine String Parameter: dir = Y
End initial condition initialize_stress_state

### Boundary Conditions

# Lithostatic pressure condition along top-side mesh (surface ID=2001)
Begin pressure
  Surface = surface_2001
  Scale Factor = 1.0
  Function = lithostatic_pressure_ytop_function
End pressure

# Lithostatic pressure condition along bottom-side mesh (surface ID=2000)
Begin pressure
Surface = surface_2000
Scale Factor = 1.0
Function = lithostatic_pressure_ybot_function
End pressure

# Fixed displacement condition along right-side mesh
Begin fixed displacement
# 
#       Components = x y z
Components = x y
Node Set = nodelist_101
End fixed displacement

# Fixed x-displacement condition along left-side mesh
Begin fixed displacement
Components = x
Node Set = nodelist_100
End fixed displacement

# Fixed x-displacement condition along right-side mesh
Begin fixed displacement
Components = x
Node Set = nodelist_102
End fixed displacement

# Fixed z-displacement condition along z=0.0 m (2D plane strain condition)
Begin fixed displacement
Components = z
Node Set = nodelist_400
End fixed displacement

# Fixed z-displacement condition along z=-1.524 m (2D plane strain condition)
Begin fixed displacement
Components = z
Node Set = nodelist_401
End fixed displacement

### Temperature Conditions
###

Begin Prescribed Temperature
Include All Blocks
Read Variable = temp
#     Copy Variable = TEMP From Model Aria_FEM
#     Receive From Transfer Field Type = NODE
End Prescribed Temperature

### Gravity
###

Begin gravity
Include all blocks
   Direction = y
Gravitational constant = 9.79
   Scale Factor = -1.0
       Function = gravitational_acceleration_function
End gravity

### Adagio Solver Parameters
###
### Adaptive Time Step definition

Begin adaptive time stepping

target iterations = 500
method = material # <solver> | material

cutback factor = 0.5
cutback factor = 1 # <0.5>
growth factor = 1.05 # <1.5>
maximum multiplier = 1e+14
minimum multiplier = 0.0001
maximum failure cutbacks = 10 # <5>
iteration window = 5 # <target_iterations/10>
End adaptive time stepping

### Solver definition ###

Begin solver

Level 1 Predictor = default # none | <default>

Begin Control Contact Adagio_CONTACT
    Level = 1
    Target Relative Residual = 0.005
    Acceptable Relative Residual = 100
    Minimum Iterations = 1
    Maximum Iterations = 1000
    Reference = EXTERNAL # <EXTERNAL> | INTERNAL | BELYTSCHKO | RESIDUAL | ENERGY
End Control Contact Adagio_CONTACT

Begin loadstep predictor
    type = scale_factor
    scale factor = 1.0 0.0
End loadstep predictor

Begin cg
    Line Search Tangent
        Target Relative Residual = 0.0005
        Acceptable Relative Residual = 0.01
        Iteration Reset = 10 # <10000>
        Iteration Print = 400
        Minimum Iterations = 1
        Maximum Iterations = 50000
        Preconditioner = diagonal # <elastic> | # block_initial |
        # probe | schur | # diagonal
        Balance Probe = 0 # <0> | 1 | 2
        Nodal Probe Factor = 1e-06 # <1.0e-06>
        Beta Method = PolakRibiere # <PolakRibiere> | # PolakRibierePlus |
        # FletcherReeves
End cg

End solver

End adagio region AdagioRegion
End adagio procedure AdagioProcedure

END SIERRA roomb_structural
APPENDIX C: SIERRA MECHANICS FOR COUPLED MULTI-PHYSICS MODELING OF SALT REPOSITORIES

SIERRA Mechanics for Coupled Multi-Physics Modeling of Salt Repositories

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ABSTRACT: The Nuclear Energy Advanced Modeling & Simulation (NEAMS) Waste Integrated Performance & Safety Code (IPSC) project is tasked to develop the “next-generation” of computational tools to model nuclear waste repositories in order to quantitatively assess the long-term performance of a disposal (or a storage) system in an engineered/geologic environment. To achieve this goal, the Waste IPSC will incorporate three levels of model fidelity: constitutive relationships derived from mechanistic sub-continuum processes; high-fidelity continuum models; and moderate-fidelity Performance Assessment (PA) continuum models. The integration of modeling and simulation capabilities at these three levels of fidelity will derive from a combination of existing code acquisition and new code development. These multi-fidelity modeling and simulation capabilities must be supported by efficient software frameworks and enabling tools/infrastructure, also derived from a combination of existing and new computer codes. Toward this end, a preliminary validation effort on high-fidelity continuum modeling was undertaken using the SIERRA Mechanics suite of codes developed by Sandia National Laboratories (Edwards & Stewart 2001) to exercise and evaluate the code suite for applicability to this class of problems.

The development of the SIERRA Mechanics code suite has been funded by the USA Department of Energy (DOE) Advanced Simulation and Computing (ASC) program for more than ten years. The goal is development of massively parallel multi-physics capabilities to support the Sandia engineering sciences mission. SIERRA Mechanics was designed and developed from its inception to run on the latest and most sophisticated, massively parallel computing hardware. It has the capability to span the hardware range from a single workstation to computer systems with thousands of processors. The foundation of SIERRA Mechanics is the SIERRA toolkit, which provides finite element application code services such as: mesh and field data management, both parallel and distributed; transfer operators for mapping field variables from one mechanics

1 INTRODUCTION

The goal of the Nuclear Energy Advanced Modeling & Simulation (NEAMS) Waste Integrated Performance & Safety Code (IPSC) project is to develop the “next-generation” of computational tools to model nuclear waste repositories through an integrated suite of multi-physics modeling and simulation capabilities to quantitatively assess the long-term performance of a disposal (or storage) system in an engineered/geologic environment (Freeze et al. 2010, Freeze et al. 2011). The Waste IPSC will provide this simulation capability for a range of disposal concepts including various waste form types, engineered barrier designs, and geologic settings; for a range of temporal and spatial scales; with appropriate consideration of the associated uncertainties; and in accordance with rigorous verification, validation, and software quality requirements.

To achieve this goal, the Waste IPSC will incorporate three levels of model fidelity: constitutive relationships derived from mechanistic sub-continuum processes; high-fidelity continuum models; and moderate-fidelity Performance Assessment (PA) continuum models.

The integration of modeling and simulation capabilities at these three levels of fidelity will derive from a combination of existing code acquisition and new code development. These multi-fidelity modeling and simulation capabilities must be supported by efficient software frameworks and enabling tools/infrastructure, also derived from a combination of existing and new computer codes. Toward this end, a preliminary validation effort on high-fidelity continuum modeling was undertaken using the SIERRA Mechanics suite of codes developed by Sandia National Laboratories (Edwards & Stewart 2001) to exercise and evaluate the code suite for applicability to this class of problems.

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the database for validation of the predictive technology that was being developed at the time for use in the licensing process (Matalucci et al. 1984). Among the pieces of the validation technology being developed then was the Multi-mechanism Deformation (MD) creep constitutive model that was eventually adopted by WIPP. The MD model, which has been migrated to and is available in the current SIERRA Mechanics toolkit, will be presented in this section. The WIPP Room D and B Thermal/Structural Interactions in-situ test configurations and the computational models that were used in this work are then described and results for those calculations are presented. Rooms B and D were chosen because they were located in the same general location within the WIPP and at the same horizon, with the major difference between them being that Room D was at ambient conditions while Room B was subjected to a significant thermal load via heaters in the floor.

2.1 Multi-mechanism deformation (MD) constitutive creep model

The Multi-mechanism Deformation (MD) creep model originally developed by Munson & Dawson (1979, 1982, 1984) and later extended by Munson et al. (1999) was used in these analyses. The MD model mathematically represents the primary and secondary creep behavior of salt due to dislocations under relatively low temperatures (compared to the melting temperature) and low to moderate stresses which are typical of mining and storage cavern operations. Three micromechanical mechanisms, determined from deformation mechanism maps (Munson 1979), are represented in the model: a dislocation climb mechanism active at high temperatures and low stresses, an empirically observed mechanism active at low temperatures and low stresses, and a dislocation slip mechanism active at high stresses. These creep mechanisms are assumed to act such that the total steady state creep rate can be written as the sum of the individual mechanism strain rates.

\[ \dot{\epsilon} = \sum \dot{\epsilon}_i \]  

(1)

The influence of temperature on the creep strain rate is included through an Arrhenius term. The steady state creep strain rates for the first and second mechanisms are identical in form and are implemented using a power law model while the third mechanism (dislocation slip) is represented using an Eyring type model.

\[ \dot{\epsilon}_s = A \left( \frac{\sigma}{C} \right)^n e^{\frac{-Q}{RT}} \]  

(2)
\[ \varepsilon_i = A_i \left( \frac{\sigma_{ii}}{G} \right)^{\kappa_i} \theta^{\frac{\phi_i}{n}} \theta^{n \sigma_{ii}} \]  

\[ \varepsilon_i = \left( B_i e^{-\alpha_i \theta} + A_i e^{-\beta_i \theta} \right) \left[ 1 + \frac{\sigma_{ii}}{G} \right] \times \exp \left( \frac{\sigma_{ii}}{\sigma_s} \right) \]  

where \( \sigma_{ii} \) is the equivalent stress, \( T \) is the temperature (absolute), \( G \) is the shear modulus, \( A_i, B_i, \alpha_i, \) and \( \beta_i \) are structure factors; \( \Omega_1 \) and \( \Omega_2 \) are activation energies; \( R \) is the universal gas constant; \( q \) is the activation volume, \( \sigma_0 \) is the stress limit, and \( H \) is the Heaviside function with argument \( \sigma_{ii} - \sigma_0 \).

From the definition of the Heaviside function, the third mechanism is only active when the equivalent stress exceeds the specified value of the stress limit \( \sigma_0 \). The equivalent stress appearing in these equations is to be the Tresca stress (Munson et al. 1980). The Tresca stress can be written in terms of the maximum and minimum principal stresses \( \sigma_1 \) and \( \sigma_3 \) respectively \( (\sigma_1 \geq \sigma_2 \geq \sigma_3) \). Alternatively, the Tresca stress may be written as a function of the Lode angle, \( \psi \), and the second invariant, \( J_2 \), of the deviatoric stress tensor, \( s \) (with components \( s_{ij} \)).

\[ \sigma_{Tresca} = \sigma_1 - \sigma_3 - 2 \cos \psi \sqrt{J_2} \]  

The Lode angle is dependent on both the second and third invariant, \( J_1 \), of the deviatoric stress tensor, \( \sigma_0 \).

\[ \psi = \frac{1}{3} \sin^{-1} \left( \frac{-3 \sqrt{J_2}}{2 J_1} \right) \quad \frac{-\pi}{6} \leq \psi \leq \frac{\pi}{6} \]  

\[ J_2 = \frac{1}{2} \varepsilon_i \varepsilon_i \]  

\[ J_3 = \frac{1}{3} \varepsilon_i \varepsilon_i \varepsilon_i \]  

The kinetic equation used in the MD model is given by Equation 9, where \( F \) is a function which accounts for transient creep effects and \( \varepsilon_i \) is the steady state dislocation creep strain rate defined by Equation 1.

\[ \varepsilon_i = F \varepsilon_i \]  

The function \( F \) has three branches: a work hardening branch \( (F > 1) \), an equilibrium branch \( (F = 1) \), and a recovery branch \( (F < 1) \).

\[ F = \begin{cases} \exp \left[ \delta \left( 1 - \frac{\varepsilon_i}{\varepsilon^*} \right) \right] & \text{\( \zeta < \varepsilon^* \) Transient Branch} \\ 1 & \text{\( \zeta = \varepsilon^* \) Equilibrium Branch} \\ \exp \left[ -\delta \left( 1 - \frac{\varepsilon_i}{\varepsilon^*} \right) \right] & \text{\( \zeta > \varepsilon^* \) Recovery Branch} \end{cases} \]  

The choice of the particular branch depends on the transient strain limit \( \varepsilon^* \) and the internal variable \( \zeta \). The transient strain limit is defined by Equation 11, where \( K_0, c, \) and \( m \) are material parameters. \( T \) is the absolute temperature, and \( G \) is the shear modulus.

\[ \varepsilon^* = K_0 T \sigma^2 \left( \frac{\sigma_n}{G} \right)^m \]  

The internal variable, \( \zeta \), appearing in the calculation of the function, \( F \), is obtained by integration of the evolution equation

\[ \dot{\zeta} = \frac{1}{F - 1} \dot{\varepsilon}_i \]  

\[ \Delta = \alpha + \beta \log \left( \frac{\sigma_n}{G} \right) \]  

\[ \delta = \alpha + \beta \log \left( \frac{\sigma_n}{G} \right) \]

2.2 Isothermal room configuration (Room D)

2.2.1 Test description and stratigraphy

The isothermal WIPP Mining Development Test (Room D) consists of a test room set into the bedded stratigraphy of the natural salt formation. The room was constructed to be thermally and structurally isolated from the other test rooms by a large pillar, approximately 79 m thick. The room has a total length of 93.3 m. The test section of the room consists of the central 74.4 m of the room and has cross section dimensions of 5.3 m wide by 3.5 m high. The Room D coordinate center is at a depth, below the ground surface, of 646.0 m. Details of the mining of the room and of the measurements that were taken are given in Munson et al. (1988). The roof of Room D follows a parting defined by a small clay seam. This seam (Clay I), along with the rest of the clay seams, and the remainder of the stratigraphy around the room are shown in Figure 1. This is the same stratigraphy used in the historical calculation of Munson et al. (1989), in which they reported agreement of the MD-model/SPECTROM-32 (2D) code combination with the Room D data. In this work, we attempted to duplicate the historical calculation as closely as possible with the MD-model/SIERRA toolset combination as an initial effort at validating SIERRA Mechanics for this class of problems.
The clay seams noted in the stratigraphy, according to Mansour et al. (1989), are not in actuality distinct seams unless associated with an anhydrite layer but are rather local horizontal concentrations of disseminated clay stringers. Therefore, computationally, seam properties can be ascribed to the concentration of clay. In the calculational model of this work, as was also the case for the historical calculation, the clay seam shear response is specified by a coefficient of friction, \( \mu = 0.2 \). Of the thirteen clay seams labeled A through M, only the nine nearest the room labeled D through L are taken as active and included in the calculation.

### 2.2.2 Configuration and computational model

The calculational model represents a slice through the center of the room length and consists of a space defined by the vertical symmetries plane through the middle of the room and by a vertical far field boundary placed far into the salt. So the model is effectively a plane strain model—which is appropriate for comparison with measurements taken at room midlength for the relatively long room. Because the SIEERRA mechanics model offers only a 3D capability, for the room calculations reported herein, the plane strain model is approximated by taking a slice (single element into the plane) to generate its 3D equivalent. The front and back faces of the resulting 3D model are then constrained against horizontal movement in the out-of-plane direction (Z-direction). The upper and lower extremes of the model are defined as shown. The boundaries, both vertical and horizontal, are sufficiently removed from the room that they cause an insignificant perturbation in stress or displacement at the room proper. Both of the vertical boundaries are constrained against horizontal (X-direction) movement, allowing only vertical displacements. The horizontal boundaries are traction (lithostatic pressure) boundaries. A uniform pressure of 15.37 MPa is applied at the upper horizontal boundary, accounting for the weight of the overburden. Krieg (1984) determined the thickness weighted average of the densities of the materials in the layers of the calculational model yielding an average density in the model of 2300 kg/m\(^3\). This density results in a uniform applied pressure of 15.97 MPa on the bottom horizontal boundary, and accounts for the presence of an instantaneously mined room.

A lithostatic initial stress state that varies linearly with depth is assumed, based on the average material density and a gravitational acceleration of 0.70 m/s\(^2\), in the model. The room surfaces are traction-free and the upper right corner of the model is fixed against horizontal and vertical (X-Y) displacements.

The finite element mesh used in the SIEERRA Mechanics calculation is not shown. However, it contains 2184 hexahedral elements and 5032 nodes.

### 2.2.3 Closure results from SIEERRA Mechanics

The Room D simulation computed the first 1100 days of creep response of the room for comparison with the Room D measurements. The simulation used the above-described computational model and MD constitutive description, with the parameters for the MD model shown in Table 1. These parameter are identical to those given in Mansour et al. 1989, in an effort to duplicate, as closely as possible, the historical calculation using SIEERRA Mechanics in place of the earlier 2D SPEC1ROM-52 code. The parameters, shown in parenthesis in Table 1 under the “Halite” heading, are the parameters for argillaceous halite that are different from those for clean halite; most parameters are the same for the two materials that were used in the calculation.
Table 1. Parameter set used for Room D calculation.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shear modulus</td>
<td>G</td>
<td>12.400</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>E</td>
<td>31.000</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td></td>
<td>0.25</td>
</tr>
<tr>
<td>Structure Factors</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Activation energies</td>
<td>Q_a</td>
<td>25.000</td>
</tr>
<tr>
<td>Universal gas constant</td>
<td>R</td>
<td>1.007</td>
</tr>
<tr>
<td>Absolute temperature</td>
<td>T</td>
<td>300</td>
</tr>
<tr>
<td>Stress tensor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stress constant</td>
<td>q</td>
<td>5.335</td>
</tr>
<tr>
<td>Transient strain limit</td>
<td>M</td>
<td>3.0</td>
</tr>
<tr>
<td>Constants</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Constants for work-</td>
<td></td>
<td></td>
</tr>
<tr>
<td>handling parameter</td>
<td>P</td>
<td>-1.05</td>
</tr>
<tr>
<td>Recovery parameter</td>
<td>e</td>
<td>0.58</td>
</tr>
</tbody>
</table>

Thus, it should be noted that the same assumptions that went into the historical calculation were also used in this one. For example, although the stratigraphy shows anhydrite and polyhalite layers, Munson et al. 1980 state: Because these layers are either sufficiently thin to be insignificant in the calculation, or are sufficiently removed from the room being simulated to be quite un-influential in the calculation, we did not include them in the calculation. Hence, the present SIERRA mechanics calculation did not include them either: instead the two materials were treated as anhydrous halite as was presumably done in the historical calculation.

It should also be noted that not all of the details of the historical calculations are well documented. Therefore, in those cases where those details are missing, we have made some assumptions, guided by expert judgment, to be able to repeat the historical calculation as closely as possible; as was the case above in treating the anhydrite and polyhalite layers as anhydrous halite rather than clean halite.

Figure 2 shows the room closure results from the mechanical simulation compared to the extensometer measurements of Room D closure. In view of the complexity of the calculation, the agreement between calculation and measurement is quite good, on the order of approximately 10% difference between them for both vertical and horizontal closure. This is of roughly the same order as the agreement seen in the historical calculation of Munson et al. 1980, and at least, in a preliminary sense, validates SIERRA Mechanics for isothermal conditions to roughly the same degree as was done for the code used in the historical calculation.

Figure 2. Comparison of calculated (SIERRA Mechanics) and measured in-situ Room D closures.

2.3 Heated room configuration (Room B)

2.3.1 Test Description and Stratigraphy

The WIPP Overtest for Simulated Defense High-Level Waste (Room B) Thermal/Structural Interactions in-situ experiment (Munson et al 1986a) is another major thermal/structural test conducted at the WIPP. It consists of a long, 93.3 m, instrumented room with a square cross-section that is 5.5 m by 5.5 m. This room has electrically heated canisters that are 0.3 m diameter by 2.39 m long (i.e., length of heated cylinders) and placed, in evenly-spaced vertical boreholes that are 0.41 m diameter by 4.9 m deep, in the floor along the room centerline. Those heaters, each with about 1.8 kW of power, were placed on 1.52 m centers to give a linear heat load of 1.18 kW/m over the central 41.2 m of the room.

Closure and temperature measurements were made during the course of the experiment in the heavily instrumented room. According to Munson et al. (1986a) closure measurements were made starting within one hour of the mining at that location and continued for the duration of the test. Three different thermocouple arrays were used to monitor the tem-
perature conditions: one for monitoring the interior canister temperatures, another that monitored the temperatures in the vicinity of the canisters; and another that monitored the temperatures in the salt around the room. The test room operated in an unheated condition initially to give a baseline room response for comparison with other similar experimental rooms (including Room D) as well as to allow time for emplacement of the heaters and construction of insulated doors at the ends of the room.

Because creep of salt is a thermally-activated process, a modest increase in temperature produces a marked acceleration in room closure rate. Room B is of identical dimensions to Room D; is in the same general vicinity and at the same depth; and has the same stratigraphy (Fig. 1).

2.3.2 Configuration and computational model
The finite element calculations used to simulate the Room B in situ experiment consisted of two separate 3D models, a thermal model and a structural model. As discussed previously for Room D, a one-element through-the-thickness model was used to mimic the plane-strain 2D models in 3D. One-way coupling between the thermal and structural responses was employed; similar to what was performed in the historical calculation of Munson et al. (1990a) using the 2D thermal code SPECTROM-41 and 2D structural code SPECTROM-32, in an effort to duplicate their calculation as closely as possible. This one-way coupling implies that thermal response was assumed to be unaffected by structural deformations. The thermal model was used to compute temperatures in the geologic formation around Room B for a simulated period of five years. The SIERRA Mechanics thermal/fluids finite element code, Aria (Notz et al. 2007), was used for this calculation. The temperatures were then used as input to the SIERRA Mechanics structural finite element code, Adagio (SIERRA Solid Mechanics Team 2010), so that thermal expansion and creep property changes induced by changes in temperature could be included in the mechanical response. Since temperature and stress gradients occur in different regions, the thermal and structural calculations required mesh refinement in different areas. As a result, the thermal and structural finite element meshes used for the Room B calculation were different, and nodal temperatures computed using the Aria calculation were interpolated to the structural mesh (Argiello et al., in prep.).

The thermal model was constructed assuming all external boundaries were adiabatic, to be consistent with the historical calculation (Munson et al. 1990b), and that the entire formation was prescribed to have an initial temperature of 300 K. The configuration remained at 300 K for the first 3.24 days and then the thermal load of 1.8 kW per canister was applied to the finite element model at the appropriate location. The discrete thermal loading from each of the canisters was simulated two-dimensionally as a uniform line source located on the left symmetry plane, extending from a depth of 3.37 m below Clay G to 5.96 m below Clay G. The thermal load for each canister was distributed over the canister spacing of 1.52 m and canister height of 2.59 m to give a uniform heat flux of 458 W/m² condition on the symmetry plane, only half of this load or 228 W/m² was applied to the thermal finite element model. A thirty year half life was simulated with a decaying exponential such that the thermal load applied along the length of the heat source had the form:

\[ q = \text{228} \exp(-7.327 \times 10^{-10} t) \]  

where \( q \) is the thermal load in W/m² and \( t \) is the time in seconds. The thermal properties of all stratigraphic materials were assumed to be the same as those for halite. Earlier work had shown that thermal responses using both an all-salt stratigraphy and a layered stratigraphy were essentially the same (see Argiello et al., in prep. for additional details). Heat transfer through the salt was modeled with a nonlinear thermal conductivity of the form:

\[ \lambda = \gamma (300/T)^7 \]  

where \( \lambda \) is the thermal conductivity, \( T \) is the absolute temperature in Kelvin, \( \gamma = 500 \) and \( \gamma = a \) are material constants. The excavated room (i.e., WIPP Room B) was treated as an "equivalent thermal material" with a conductivity allowing radiation heat transfer in the room to be simulated by conduction. This approximate method of modeling radiation was used in the WIPP Benchmark II numerical simulation activity (Morgan et al. 1991), and the properties of the "equivalent thermal material" were chosen so that the thermal response computed with this material is almost the same as the response computed by modeling radiation in the room. Note that the "equivalent thermal material" was not included in the structural model mesh. The thermal properties of halite and the "equivalent thermal material," used in this simulation are presented in Table 2.

<table>
<thead>
<tr>
<th>Table 2. Thermal properties used in Room B thermal simulations using Aria.</th>
<th>( \lambda ) (W/mK)</th>
<th>( \gamma ) (K/°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material</td>
<td>Face</td>
<td>Equivalent thermal material</td>
</tr>
<tr>
<td>Density, ( \rho ) (kg/m³)</td>
<td>2300</td>
<td>1</td>
</tr>
<tr>
<td>Specific heat, ( c_p ) (J/kgK)</td>
<td>860</td>
<td>1000</td>
</tr>
<tr>
<td>Coefficient of linear thermal expansion, ( \alpha ) (K⁻¹)</td>
<td>45×10⁻⁶</td>
<td>N/A</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>5</td>
<td>50</td>
</tr>
<tr>
<td>Parameter</td>
<td>1.14</td>
<td>0</td>
</tr>
</tbody>
</table>
The halite thermal property values were taken from the original WIPP reference property set, as described by Krieg 1984, for halite and the properties for the "equivalent thermal material" are the same as those used in Benchmark II (Morgan et al. 1981). Lastly, the thermal loss from the room was modeled by a convective boundary at the WIPP room B surfaces using Newton’s law of cooling as:

\[ q' \cdot n = h(T - 300) \]  

(17)

where \( q' \) is the thermal flux vector, \( n \) is the outward normal unit vector, \( h \) is the convective heat transfer coefficient, and \( T \) is the surface temperature in Kelvin. The convective boundary acts as a heat sink whenever the temperature on the room surface exceeds the initial 300 K temperature. Thus, as the room surface temperature rises, the rate of heat loss increases. Because the convective heat transfer coefficient was unknown, it was adjusted prior to any structural calculations until a suitable value (0.18 W/m²K) was determined to give agreement with the measured temperatures reported above and below the WIPP Room B, similar to what was done in the historical calculation. Note that insulated doors were constructed at the entries of Room B to prevent the circulation of ventilation air from the rest of the mine; nonetheless, there was still a marked heat loss through these doors (Munson et al. 1990b).

With the exception of some material properties and the fact that the model is now subjected to heat loading, the mechanical computational model for Room B is, for all practical purposes, almost identical to the model used for Room D. It has been described in the previous sub-section and will not be repeated here. Only the subler differences are discussed, including the behavior of the non-salt materials. The anhydrite and polyhalite regions are now modeled as separate materials, as was done in the historical calculation of Munson et al. 1990a. The anhydrite and polyhalite materials are modeled using a Drucker-Prager constitutive model to treat elastic and inelastic behavior. The mechanical responses of the anhydrite and polyhalite materials were treated elastically until yielding occurs, but once the yield stress is reached, plastic strain accumulates. The Drucker-Prager criterion can be written as:

\[ J_2 = c - a \mu \]  

(18)

where \( J_2 \) is the modified second deviatoric stress invariant (i.e., \( J_2 = \sqrt{\mu} \)), \( c \) & \( \mu \) are constants, and \( \mu \) is the first stress invariant. Values of \( c = 1.35 \) MPa and \( \mu = 0.45 \) were used for the anhydrite and \( c = 1.42 \) MPa and \( \mu = 0.475 \) were used for the polyhalite in the Room B calculation. In addition, the value of the MD Model parameter, \( \chi_0 \), previously used for argillaceous halite in Room D has now also been modified, as was also done in the historical calculation. A value of \( \chi_0 = 1.783 \times 10^6 \) is used for the Room B argillaceous halite.

2.3.3 Thermal and closure results from SIERRA Mechanics

In the interest of brevity, only a few results from the Room B calculation are presented here to illustrate the validity of SIERRA Mechanics for this class of problems. Many more details on this calculation, as well as for the isothermal Room D calculation, can be found elsewhere (Argiello et al., in prep.).

Figure 3 shows the computed thermal response for a series of six points extending from immediately adjacent to the roof of the room up some distance vertically into the host rock, as indicated by the numbers in parenthesis shown in the legend of the figure, where these numbers, 15.2, 9.1, etc., are in units of meters. These locations correspond to measurement locations probe by the B_745 thermocouple unit (Munson et al. 1990b). It is apparent that, in general, the agreement between calculation and data is better away from the room surface. However, even for the closer-in locations, the agreement is still relatively good, with only a few degrees difference.

![Figure 3. Comparisons of measured in-situ Room B temperatures from thermocouple unit B_745 with computed results from SIERRA Mechanics.](image)

Similarly, Figure 4 shows the computed thermal response for a series of points extending from immediately adjacent to the floor of the room down some distance off-vertically into the host rock, per the numbers in parenthesis shown in the legend of the figure. These locations correspond to measurement locations probe by the B_705 thermocouple unit (Munson et al. 1990b). At these locations, the agreement between calculation and data is quite good overall. This general trend of acceptable agreement, pervaded throughout the other thermocouple units where comparisons were made, with agreement at some locations better than at others.
Figure 5 shows the room closure results from the thermo-mechanical simulation compared to the extensometer measurements of Room B closure, measured at room midwidth and midheight. Again, in view of the complexity of the calculation, the agreement between calculation and measurement is quite good, with an under-prediction of horizontal and vertical closures of less than 1% and approximately 1%, respectively, at 1000 days. This is roughly the same order as the agreement seen in the historical calculation of Munson et al. (1989), and once again, in a preliminary sense, validates SIERRA Mechanics for non-isothermal conditions to roughly the same degree as was done for the codes used in the historical calculation. It should be noted that, from their historical calculation, Munson et al. (1990a) thought that “the large discrepancy between the calculated and measured vertical closure is believed to be due to a direct consequence of fracture and separation in the immediate roof” because the MD model, as presented above, is not capable of modeling those features, we concur with their assessment and believe that such capability, among others, should be pursued in any future advanced salt constitutive model developed for incorporation into SIERRA Mechanics for modeling the next generation of repository systems in salt.

3 LARGE 3D DEMONSTRATION PROBLEM

A study was recently performed of a generic salt repository (GSR) for disposal of wastes generated by a conventional spent nuclear fuel recycling facility (Stone et al. 2010). Because the in-situ tests discussed previously are relatively small computational problems it was desirable to demonstrate the SIERRA Mechanics toolset applied to a more challenging computational model of a more realistic size that could be more typical of the problem size that will need to be solved for future repository systems. Furthermore, although complex, the previously described in-situ thermal-mechanical problem only exercised the code suite in a one-way coupled mode and it was desirable to demonstrate that the toolset can solve more fully coupled-physics problems. Finally, it was also desirable to demonstrate the SIERRA Mechanics capability on a truly 3D configuration, typical of what will be needed in next generation tools applied to a repository setting.

The GSR study proposed a disposal strategy in which a series of panels is constructed underground. Each panel consists of individual rooms, with each room containing many alcoves. The disposal strategy assumes placement of one waste package at the end of each alcove, to be covered by crushed salt backfill for radiation-shielding of personnel accessing adjacent alcoves. The backfill effectively insulates the waste package, locally increasing waste package and near-field repository temperatures. The thermal output for each vitrified borosilicate glass waste canister is 8,400 W and decays to approximately 30% original power output after 50 years.

A coupled thermal-mechanical analysis of the salt repository was performed using the SIERRA Mechanics code suite. The goals of the analysis were to determine the peak intact salt temperature over time and to characterize the closure response of the alcove including the change in porosity of the crushed salt backfill. A 3D finite element model of a single storage alcove and haulage-way was developed utilizing planes of symmetry through the alcove and adjacent haulage-way. Two different analysis domains and mesh discretizations were utilized: one for the thermal analysis and a different discretization for the geomechanics analysis. Figure 6 shows a close-up of the mesh used for the geomechanical analysis. Field transfer operators in the SIERRA toolkit were used to pass interpolated nodal tempora
ture and displacement data between the different (thermal and mechanical) domains. This simulation was run using 96 processors and took approximately 96 hours per processor to complete compared to less than ten of hours on a single processor for the in-situ test calculations described earlier.

Some of the discriminating features of this highly nonlinear thermal-mechanical analysis included the use of thermal contact surfaces to model the effect of room closure on the thermal conduction that occurs as the room surfaces deform and come into contact. The mechanical effect of the large salt creep deformation was also captured through the use of contact surfaces in the mechanical calculation. The effect of thermal radiation between heated surfaces within the alcove and haulage-way was also modeled within SIERRA Mechanics using the capability to recompute the radiation view factors as the surfaces deform (in radiative heat transfer, a radiation view factor monitors the fraction of energy leaving one surface and arriving at another surface). Unlike in the previous in-situ test calculations, the use of an "equivalent" material for thermally modeling the room was not needed. The mechanical response of the salt was modeled using both a Norton power law secondary creep model and the MD model described earlier. The compaction behavior of the crushed salt backfill was modeled with a nonlinear pressure versus volume-strain relationship.

The details of this simulation, as well as results of both the thermal and mechanical analyses, are presented in Stone et al. 2010. Here we include only select results that demonstrate the complex threedimensional room-closure behavior. The need for the large deformation, large strain mechanics formulation is clearly shown by the magnitude of the deformation (Fig. 7). The crushed salt backfill develops a non-uniform porosity with most of the compaction occurring near the roof of the alcove (Fig. 8). This variation of compaction of the backfill from higher at the roof to lower near the floor is in qualitative agreement with measurements of porosity in the backfill seen in experiments (Becuhold et al. 2009).

4 SUMMARY & CONCLUSIONS

Herein, results from a systematic study have been presented in which the SIERRA Mechanics code suite was exercised on a set of salt repository problems, including the isothermal Room D and the heated Room B in-situ experiments at the WIPP. This was done to validate its applicability to this class of problems and to further demonstrate its use on anticipated more complex coupled simulations of future nuclear waste salt repositories.

Results shown indicate that, in view of the complexity of the calculations used for the two in-situ experiments, the agreement between the SIERRA
Mechanics calculations and measurements is quite good, roughly the same order as the agreement seen previously in the historical calculations. Therefore, in a preliminary sense, these two simulations of insitu experiments at the WIPP validate SIERRA Mechanics to roughly the same degree as done previously. However, modern verification & validation and uncertainty quantification practices are likely to place significantly more stringent requirements on such computational tools to deem them acceptable, in a regulatory sense, for future nuclear waste repositories in salt. The demonstration GSR calculation has shown the applicability of SIERRA Mechanics to large-scale parallel computational problems that are likely to be the norm in assessing future repositories. This code suite is an example of a valuable toolset for use on the NEAMS Waste IPSC project or one with the capabilities that can be developed as the disposal community ventures into the next generation of repository computational tools.

ACKNOWLEDGEMENTS

We wish to acknowledge James Bean for his many contributions to this effort, John Holland for his contributions on the GSR calculation, and DOE NE NEAMS program for supporting this work. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

REFERENCES


APPENDIX D: SIERRA MECHANICS COUPLING SYNTAX AND DESCRIPTION

A crucial and necessary method used to permit the numerical coupling between two different computational meshes (i.e., a thermal mesh and a structural mesh), was accomplished through the use of the SIERRA Mechanics transfer syntax commands defined in the Arpeggio input deck as:

```
Begin Transfer Aria_to_Adagio
  Interpolate Volume Nodes from AriaRegion to AdagioRegion
  Nodes Outside Region are ignore
  Send Field Solution->Temperature State New to Temperature State New
  Search Coordinate Field model_coordinates state none to model_coordinates state none
  Send Block block_1 to block_1 block_2 block_3 block_4
End Transfer Aria_to_Adagio

Begin Transfer Adagio_to_Aria
  Interpolate Volume Nodes from AdagioRegion to AriaRegion
  Nodes Outside Region are ignore
  Send Field Displacement State New to Solution->Mesh_Displacements State New
  Search Coordinate Field model_coordinates state none to model_coordinates state none
  Send Block block_1 block_2 block_3 block_4 to block_1
End Transfer Adagio_to_Aria
```

where the thermal mesh has two materials (or block identifiers: 1 and 2) and the structural mesh has four materials (or block identifiers: 1, 2, 3, and 4). The thermal mesh material Id. #2 is the equivalent thermal material. Thus, no displacement data from the structural mesh was allowed to be transferred to the thermal mesh material Id #2, as seen above, using the syntax instructions: "Send Block block_1 block_2 block_3 block_4 to block_1" in the "Begin Transfer Adagio to Aria" command section. Likewise, no temperature data was allowed to be transferred from the thermal mesh to the structural mesh, as seen above, using the syntax instructions: "Send Block block_1 to block_1 block_2 block_3 block_4" in the "Begin Transfer Adagio to Aria" command section. Proper and careful use of the SIERRA Mechanics transfer operator language (i.e., syntax) is the computational bridge that successfully accomplishes coupling different physics.
APPENDIX E: HEATED ROOM COUPLED CALCULATION #1
(EQUIVALENT THERMAL MATERIAL) INPUT DECK

# directory: /scratch/jsrath/NEAMS/roomb/coupled/simu1000
# file: arpeggio.i
# author: Jonathan Scott Rath
# description: UFD 2012 WIPP Room B input deck
# UFD = Used Fuels Disposition
# WIPP = Waste Isolation Pilot Plant = WIPP
# SIERRA = Sandia Integrated Environment for Robust
# Research Algorithms
# SIERRA Thermal-Mechanical (Aria-Adagio) Calculation
# SIERRA TM WIPP Room B Two-Way Coupled Calculation
# Model 3 (Room B, Thermal+Mechanical)

# revision_log: 10/AUGUST/2012
# - Adapted to repeat un-coupled FY2011 NEAMS
# - Aria/Adagio Equivalent Thermal Material model
# : 06/AUGUST/2012
# - Shifted Dirichlet Temperature B.C. for DHLW power
# on time (325 days of unheated, T=300 Kelvin)
# : 01/AUGUST/2012
# - Modified for Dirichlet Temperature B.C. on ROOM B
# : 22/MARCH/2012
# - Added material AIR
# - Modified for Dirichlet Temperature B.C. on ROOM B
# : 09/MARCH/2012
# - Modified time stepping for Adagio and Aria region
# : 01/MARCH/2012
# - Implemented new Sam Subia advised Enclosure
# Radiation approach and method utilizing partial
# enclosure constructs, etc.
# : 29/FEBRUARY/2012
# - Adapted new syntax for THERMAL STRAIN X FUNCTION
# - Adapted new syntax for THERMAL STRAIN Y FUNCTION
# - Adapted new syntax for THERMAL STRAIN Z FUNCTION
# - Using THERMAL LOG STRAIN X FUNCTION
# - Using THERMAL LOG STRAIN Y FUNCTION
# - Using THERMAL LOG STRAIN Z FUNCTION
# - Adapted heat flux at Room B opening to account
# for normal outward direction
# - Added convection heat transfer boundary condition
# (Side Set 4000, h=0.51 W/m^2/K)
# - Added 3dHex8_MESH & 3dHex27_MESH variable control
# - Added non-conditional function tpf.include
# - Added non-conditional function ntc.include
# - Added coefficient of thermal expansion
# - Added power law thermal conductivity form
# - First Edition for "TM"

# unit system: System International (SI)
# mass = kilogram (kg)
# length = meter (m)
# time = seconds (sec)
# Temperature = Kelvin
# density = kg/(m^3)
# velocity = meter/sec = 10^-3*km/sec
# acceleration = m/(sec^2)
# force = mass * acceleration = kg*m/sec^2
# pressure = Newton / (m^2)
# = Pascal
# energy = Newton*m
# = Joule
BEGIN SIERRA WIPP_Room_B_Thermal_Structural_Funded_By_UFD

Begin diagnostic control Adagio_Diagnostics
enable "tangent"
End diagnostic control Adagio_Diagnostics

title UFD WIPP Room B Coupled Thermal-Structural Response Simulation

define direction x with vector 1.0 0.0 0.0
define direction y with vector 0.0 1.0 0.0
define direction z with vector 0.0 0.0 1.0

define direction dir_1 with vector 0.7071067812 0.0 0.7071067812
define direction dir_2 with vector -0.7071067812 0.0 -0.7071067812

define point origin with coordinates 0.0 0.0 0.0

BEGIN GLOBAL CONSTANTS
Stefan Boltzmann Constant = 5.67e-08 \[\text{watt (Nm/s)}/(\text{meter}^2*\text{degK}^4)\]
End

BEGIN FUNCTION DEFINITIONS

Begin definition for function DHLW_power_flux_function
Abscissa = time \[\text{second}\]
Ordinate = DHLW_power_flux \[\text{watt (Nm/s)}]/(\text{meter}^2)\]
Type = analytic
Evaluate Expression = "x <= 28080000 ? 0.0 : 228.012039*exp(-7.327e-10*x);"
Differentiate Expression is "x <= 28080000 ? 0.0 : -1.67064421e-07*exp(-7.327e-10*x);"
End definition for function DHLW_power_flux_function

Begin definition for function gravitational_acceleration_function
Type is piecewise linear
Begin values
0 1
157784630.4 1
End values
End definition for function gravitational_acceleration_function

Begin definition for function lithostatic_pressure_ybot_function
Type is piecewise linear
Begin values
0 157784630.4
157784630.4 15780670.02
End values
End definition for function lithostatic_pressure_ybot_function

Begin definition for function lithostatic_pressure_ytop_function
Type is piecewise linear
Begin values
0 13570000
157784630.4 13570000
End definition for function lithostatic_pressure_ytop_function
End definition for function lithostatic_pressure_ytop_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 2.4e-05 [1/Kelvin]
# ---------------------------------
# T_ref 0.0
# T_max (T_max-T_ref)*alpha
# ---------------------------------

Begin definition for function polyhalite_thermal_strain_function
  Type is piecewise linear
  Begin values
  300 0
  1500 0.0288
  End values
End definition for function polyhalite_thermal_strain_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 4e-05 [1/Kelvin]
# ---------------------------------
# T_ref 0.0
# T_max (T_max-T_ref)*alpha
# ---------------------------------

Begin definition for function argillaceous_thermal_strain_function
  Type is piecewise linear
  Begin values
  300 0
  1500 0.048
  End values
End definition for function argillaceous_thermal_strain_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 2e-05 [1/Kelvin]
# ---------------------------------
# T_ref 0.0
# T_max (T_max-T_ref)*alpha
# ---------------------------------

Begin definition for function anhydrite_thermal_strain_function
  Type is piecewise linear
  Begin values
  300 0
  1500 0.024
  End values
End definition for function anhydrite_thermal_strain_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 4.5e-05 [1/Kelvin]
# ---------------------------------
# T_ref 0.0
# T_max (T_max-T_ref)*alpha
# ---------------------------------

Begin definition for function halite_thermal_strain_function
  Type is piecewise linear
  Begin values
  300 0
  1500 0.054
  End values
End definition for function halite_thermal_strain_function
Begin definition for function polyhalite_pressure_volstrain_function
Type is piecewise linear
Ordinate is volumetric_strain
Abscissa is Pressure
Begin values
-1 -6.583333333e+10 # -65833.33333 MPa
0 0
1 6.583333333e+10 # 65833.33333 MPa
End values
End definition for function polyhalite_pressure_volstrain_function

Begin definition for function anhydrite_pressure_volstrain_function
Type is piecewise linear
Ordinate is volumetric_strain
Abscissa is Pressure
Begin values
-1 -8.344444444e+10 # -83444.44444 MPa
0 0
1 8.344444444e+10 # 83444.44444 MPa
End values
End definition for function anhydrite_pressure_volstrain_function

#################################################
################ ELEMENT SECTIONS ###############
#################################################

Begin solid section hex8
Strain Incrementation = midpoint_increment
Hourglass rotation = scaled
End solid section hex8

#################################################
################# MATERIAL MODELS ###############
#################################################

Begin Property Specification for material polyhalite
Density = 2300
thermal log strain x function = polyhalite_thermal_strain_function
thermal log strain y function = polyhalite_thermal_strain_function
thermal log strain z function = polyhalite_thermal_strain_function
Begin parameters for model soil_foam
youngs modulus = 5.53e+10 # [Pa]
poissons ratio = 0.36 # [dimensionless]
# bulk modulus = 6.583333333e+10 # [Pa]
# shear modulus = 2.033088235e+10 # [Pa]
a0 = 2459512.147 # [Pa]
a1 = 2.457780096
a2 = 0 # [1/Pa]
prom pressure cutoff = -1000704.722 # [Pa]
prom pressure function = polyhalite_pressure_volstrain_function
End Parameters for model soil_foam
End Property Specification for material polyhalite

Begin Property Specification for material argillaceous
Density = 2300
thermal log strain x function = argillaceous_thermal_strain_function
thermal log strain y function = argillaceous_thermal_strain_function
thermal log strain z function = argillaceous_thermal_strain_function
Begin Parameters For Model MD_Creep
# Youngs Modulus = 3.100000833e+10
# Poissons Ratio = 0.250000336
# Lambda = 1.240003333e+10
# Two Mu = 2.48e+10

End Property Specification for material argillaceous
Bulk Modulus = 2.06667e+10
Shear Modulus = 1.24e+10
   A1 = 1.406e+23
   Q1/R = 12581.78
# Q1/RT = 41.39296667 # Isothermal, T=300 Kelvin
   N1 = 5.5
   B1 = 8993300
   A2 = 1.3131e+13
   Q2/R = 5032.71
# Q2/RT = 16.7757 # Isothermal, T=300 Kelvin
   N2 = 5
   B2 = 0.042875
Sig0 = 20570000
Q1c = 5335
M = 3
K0 = 2470000
# CSTAR = 0.009189
# TK = 300
# C = 2.759 # C = CSTAR/TK (MD Creep model uses C when
# isothermal)
C = 0.009189 # C (MD Creep model uses C=CSTAR when
nonisothermal)
   Alpha = -14.96
   Beta = -7.738
   Delta1c = 0.58
   Amul = 0.5
   Grwfac = 1.05
   Epstol = 0.005
   Shkfac = 1
   Itype = 0
   Angle = 0.1
End Parameters For Model MD_Creep
End Property Specification for material argillaceous

Begin Property Specification for material anhydrite
   Density = 2300
   thermal log strain x function = anhydrite_thermal_strain_function
   thermal log strain y function = anhydrite_thermal_strain_function
   thermal log strain z function = anhydrite_thermal_strain_function
   Begin parameters for model soil_foam
      youngs modulus = 7.51e+10 # [Pa]
      poissons ratio = 0.35 # [dimensionless]
#      bulk modulus = 8.3444444444e+10 # [Pa]
#      shear modulus = 2.78148148148e+10 # [Pa]
      a0 = 2338268.59 # [Pa]
      a1 = 2.33826859
      a2 = 0 # [1/Pa]
      pressure cutoff = -1000000 # [Pa]
      pressure function = anhydrite_pressure_volstrain_function
   End Parameters for model soil_foam
End Property Specification for material anhydrite

Begin Property Specification for material halite
   Density = 2300
   thermal log strain x function = halite_thermal_strain_function
   thermal log strain y function = halite_thermal_strain_function
   thermal log strain z function = halite_thermal_strain_function
   Begin Parameters For Model MD_Creep
#      Youngs Modulus = 3.1e+10
#      Poissons Ratio = 0.25
#      Lambda = 1.24e+10
#      Two Mu = 2.48e+10
      Bulk Modulus = 2.066666667e+10
Shear Modulus = 1.24e+10
A1 = 8.386e+22
Q1/R = 12581.78158
# Q1/RT = 41.93927193 # Isothermal, T=300 Kelvin
N1 = 5.5
B1 = 6086000
A2 = 9.672e+12
Q2/R = 5032.712632
# Q2/RT = 16.77570877 # Isothermal, T=300 Kelvin
N2 = 5
B2 = 0.03034
Sig0 = 20570000
Qlc = 5335
M = 3
K0 = 627500
# CSTAR = 0.009189
# TK = 300
# C = 2.759 # C = CSTAR/TK (MD Creep model uses C when isothermal)
C = 0.009189 # C (MD Creep model uses C=CSTAR when nonisothermal)
Alpha = -17.37
Beta = -7.738
Delta = 0.58
Amult = 0.5
Grwfac = 1.05
Epstol = 0.005
Shkfac = 1
Itype = 0
Angle = 0.1
End Parameters For Model MD_Creep
End Property Specification for material halite
# Material ONE ("Halite")
Begin Aria Material ONE
Density = Constant Rho = 2300 # [kg/m^3]
Thermal Conductivity = Power_law A = 3333.406168 gamma = -1.14
Specific heat = Constant Cp = 860 # [joule (Nm)]/(kilogram*degK)
Emissivity = Constant e = 0.8 # [1]
Heat Conduction = basic
End Aria Material ONE
# Material TWO ("Thermal Equivalent Material")
Begin Aria material TWO
Density = Constant Rho = 1 # [kg/m^3]
Thermal Conductivity = Constant k = 50 # [watt (Nm/s)]/(meter*degK)
Specific Heat = Constant Cp = 1000 # [joule (Nm)]/(kilogram*degK)
Heat Conduction = basic
End Aria material TWO

################################################
############## FINITE ELEMENT MODELS ##############
################################################

Begin Finite Element Model Adagio_FEM
Database Name = roomb.g
Database Type = exodusII
Begin parameters for block block_1
material polyhalite
solid mechanics use model soil_foam
section = hex8
hourglass stiffness = 0.003
End Parameters for block block_1

Begin parameters for block block_2
material argillaceous
solid mechanics use model MD_Creep
section = hex8
hourglass stiffness = 0.003
End Parameters for block block_2

Begin parameters for block block_3
material anhydrite
solid mechanics use model soil_foam
section = hex8
hourglass stiffness = 0.003
End Parameters for block block_3

Begin parameters for block block_4
material halite
solid mechanics use model MD_Creep
section = hex8
hourglass stiffness = 0.003
End Parameters for block block_4

End Finite Element Model Adagio_FEM

Begin Finite Element Model Aria_FEM

Database Name = roombq.g
Database Type = exodusII
Coordinate System is Cartesian

Use Material ONE for block_1
Use Material TWO for block_2

End Finite Element Model Aria_FEM

#################################################
############# LINEAR SOLVERS ###################
#################################################

Begin Aztec Equation Solver AriaLinearEquationSolverAztec
Solution Method = cg
Preconditioning Method = DD-ICC
Maximum Iterations = 500
Residual Norm Tolerance = 1e-08
Residual Norm Scaling = r0
End Aztec Equation Solver AriaLinearEquationSolverAztec

Begin Trilinos Equation Solver AriaLinearEquationSolverTrilinos
Solution Method = cg
Preconditioning Method = multilevel #jacobi
Maximum Iterations = 2000
Residual Norm Scaling = r0
Residual Norm Tolerance = 1.0e-08
End Trilinos Equation Solver AriaLinearEquationSolverTrilinos

#################################################
############ ARPEGGIO PROCEDURE ###################
#################################################
Begin Procedure arpeggio_procedure

Begin Solution Control Description
Use System Main

Begin System Main
Simulation Start Time = 0
Simulation Termination Time = 157784630.4 # 5 [years] = 1826.211 [days]

Simulation Max Global Iterations = 1e+12
Begin Transient Time_Block_1
Advance AriaRegion
Transfer Aria_to_Adagio
Advance AdagioRegion
Transfer Adagio_to_Aria
End Transient Time_Block_1
Begin Transient Time_Block_2
Advance AriaRegion
Transfer Aria_to_Adagio
Advance AdagioRegion
Transfer Adagio_to_Aria
End Transient Time_Block_2
End System Main

Begin Parameters For Transient Time_Block_1
Start Time = 0
Termination Time = 28080000 # 0.8898205081 [years] = 325 [days]
Begin Parameters For Aria Region AriaRegion
    Time Integration Method = Second_Order
    Time Step Variation = Adaptive
    Initial Time Step Size = 1e-06
    Minimum Time step Size = 5e-07
    Maximum Time step Size = 26055 # 0.00082565076 [years] = 0.3015625 [days]
    Maximum Time Step Size ratio = 10
    Minimum Resolved Time Step Size = 5e-07
    Predictor-Corrector Tolerance = 0.0005
    Predictor-Corrector Normalization = MAX
End Parameters for Aria Region AriaRegion
Begin parameters for Adagio Region AdagioRegion
    Time Increment = 1e-06
End Parameters for Adagio Region AdagioRegion
End Parameters for Transient Time_Block_1

Begin Parameters For Transient Time_Block_2
Start Time = 28080000 # 0.8898205081 [years] = 325 [days]
Termination Time = 157784630.4 # 5 [years] = 1826.211 [days]
Begin Parameters For Aria Region AriaRegion
    Time Integration Method = Second_Order
    Time Step Variation = Adaptive
    Initial Time Step Size = 100 # 3.168876454e-06 [years] = 0.001157407407 [days]
    Minimum Time step Size = 50
    Maximum Time step Size = 864000 # 0.02737909256 [years] = 10 [days]
    Maximum Time Step Size ratio = 10
    Minimum Resolved Time Step Size = 50
    Predictor-Corrector Tolerance = 0.0005
    Predictor-Corrector Normalization = MAX
End Parameters for Aria Region AriaRegion
Begin parameters for Adagio Region AdagioRegion
    Time Increment = 100 # 3.168876454e-06 [years] = 0.001157407407 [days]
End Solution Control Description

#########################################################################
######## SIERRA CODE TO CODE TRANSFERS #########
#########################################################################

Begin Transfer Aria_to_Adagio
  Interpolate Volume Nodes from AriaRegion to AdagioRegion
  Nodes Outside Region are ignored
  Send Field Solution->Temperature State New to Temperature State New
  Search Coordinate Field model_coordinates state none to model_coordinates
  state none
  Send Block block_1 block_2 block_3 block_4
End Transfer Aria_to_Adagio

Begin Transfer Adagio_to_Aria
  Interpolate Volume Nodes from AdagioRegion to AriaRegion
  Nodes Outside Region are ignored
  Send Field Displacement State New to Solution->Mesh_Displacements State New
  Search Coordinate Field model_coordinates state none to model_coordinates
  state none
  Send Block block_1 block_2 block_3 block_4 to block_1
End Transfer Adagio_to_Aria

#########################################################################
############ ARIA REGION ############
#########################################################################

Begin Aria Region AriaRegion
  Use Finite Element Model Aria_FEM
  Use Linear Solver AriaLinearEquationSolverAztec
  Nonlinear Solution Strategy = Newton
  NONLINEAR RESIDUAL TOLERANCE = 1.0e-6
  MAXIMUM NONLINEAR ITERATIONS = 5
  NONLINEAR RELAXATION FACTOR = 1.0
  Use DOF Averaged Nonlinear Residual
  Accept Solution After Maximum Nonlinear Iterations = true

#########################################################################
##### GOVERNING EQUATIONS #####
#########################################################################

#SRC
EQ Energy for Temperature        On All_blocks Using Q1 with Lumped_Mass DIFF
EQ Mesh   for Mesh_Displacements On block_1    Using Q1 with Xfer
#   EQ Mesh   for Mesh_Displacements On block_2    Using Q1 with Diff
PostProcess HEAT_FLUX on All_Blocks using Q1

#########################################################################
##### THERMAL INITIAL CONDITIONS #####
#########################################################################

IC CONST  on All_blocks  Temperature = 300

#########################################################################
##### THERMAL BOUNDARY CONDITIONS #####
#########################################################################
# Adiabatic or Isentropic BC (i.e., "von Neuman") energy flux = 0

# von Neuman B.C. left symmetry
BC Flux for Energy on surface_1000 = constant flux = 0.0

# von Neuman B.C. right far-field
BC Flux for Energy on surface_1001 = constant flux = 0.0

# von Neuman B.C. y-vertical bottom model
BC Flux for Energy on surface_2000 = constant flux = 0.0

# von Neuman B.C. y-vertical top model
BC Flux for Energy on surface_2001 = constant flux = 0.0

# Convective heat transfer, \( q = H \times (T - T_{REF}) \)

# Heat Flux due to natural heat convection (WIPP room heat loss)
BC Flux for Energy on surface_4000 = Nat_Conv \( T_{REF} = 300 \) \( H = 0.18 \)

# BC Flux for Energy on surface_6666 = Function Name = DHLW_power_flux_function

Begin Heat Flux Boundary Condition Aria_DHLW
Add Surface surface_6666
Flux Time Function = DHLW_power_flux_function
End Heat Flux Boundary Condition Aria_DHLW

Begin Results Output output_Aria
Database Name = roombq.e
Database Type = ExodusII
Global Variables = time_step as timestep
Nodal Variables = solution->mesh_displacements as displ
Nodal Variables = solution->temperature as temp
Nodal Variables = pp->HEAT_FLUX as heatflux
Timestep Adjustment Interval = 4
At time 0, Increment = 604800 # ( t=0 seconds, incr=1 weeks )
At time 15778463.04, Increment = 2629743.84 # ( t=0.5 years, incr=1 months )
At time 31556926.08, Increment = 2629743.84 # ( t=1 years, incr=1 months )
At time 63113852.16, Increment = 2629743.84 # ( t=2 years, incr=1 months )
At time 94670778.24, Increment = 2629743.84 # ( t=3 years, incr=1 months )
At time 126227704.3, Increment = 2629743.84 # ( t=4 years, incr=1 months )
At time 157784630.4, Increment = 2629743.84 # ( t=5 years, incr=1 months )
Termination Time = 157784630.4 # 5 years
End Results Output output_Aria

Begin History Output history_output_Aria
Database Name = roombq.h
Database Type = ExodusII
At time 0, Increment = 604800 # ( t=0 seconds, incr=1 weeks )
At time 15778463.04, Increment = 2629743.84 # ( t=0.5 years, incr=1 months
)
At time 31556926.08, Increment = 2629743.84 # ( t=1 years, incr=1 months )
At time 63113852.16, Increment = 2629743.84 # ( t=2 years, incr=1 months )
At time 126227704.3, Increment = 2629743.84 # ( t=4 years, incr=1 months )
At time 157784630.4, Increment = 2629743.84 # ( t=5 years, incr=1 months )
Termination Time = 157784630.4 # 5 years
Node solution->temperature Nearest Location   0.0   -1.08  -0.762  as A1
Node solution->temperature Nearest Location   0.0   -1.54  -0.762  as A2
Node solution->temperature Nearest Location   0.0   -1.99  -0.762  as A3
Node solution->temperature Nearest Location   0.0   -2.38  -0.762  as A4
Node solution->temperature Nearest Location   0.0   -2.91  -0.762  as A5
Node solution->temperature Nearest Location   0.0   -3.29  -0.762  as A6
Node solution->temperature Nearest Location   0.0   -4.20  -0.762  as A7
Node solution->temperature Nearest Location   0.0   -5.12  -0.762  as A8
Node solution->temperature Nearest Location   0.0   -5.96  -0.762  as A9
Node solution->temperature Nearest Location   0.0   -6.03  -0.762  as A10
Node solution->temperature Nearest Location   0.0   -6.95  -0.762  as A11
Node solution->temperature Nearest Location   0.0   -10.22 -0.762  as A12
Node solution->temperature Nearest Location   0.0   -16.32 -0.762  as A13
Node solution->temperature Nearest Location   0.15  -1.08  -0.762  as B1
Node solution->temperature Nearest Location   0.15  -3.37  -0.762  as B2
Node solution->temperature Nearest Location   0.15  -4.01  -0.762  as B3
Node solution->temperature Nearest Location   0.15  -4.65  -0.762  as B4
Node solution->temperature Nearest Location   0.15  -5.32  -0.762  as B5
Node solution->temperature Nearest Location   0.15  -5.96  -0.762  as B6
Node solution->temperature Nearest Location   0.21  -1.08  -0.762  as C1
Node solution->temperature Nearest Location   0.21  -2.38  -0.762  as C2
Node solution->temperature Nearest Location   0.21  -3.29  -0.762  as C3
Node solution->temperature Nearest Location   0.21  -4.20  -0.762  as C4
Node solution->temperature Nearest Location   0.21  -5.12  -0.762  as C5
Node solution->temperature Nearest Location   0.21  -6.03  -0.762  as C6
Node solution->temperature Nearest Location   0.21  -6.95  -0.762  as C7
Node solution->temperature Nearest Location   0.40  -1.08  -0.762  as D1
Node solution->temperature Nearest Location   0.40  -2.38  -0.762  as D2
Node solution->temperature Nearest Location   0.40  -3.29  -0.762  as D3
Node solution->temperature Nearest Location   0.40  -4.20  -0.762  as D4
Node solution->temperature Nearest Location   0.40  -5.12  -0.762  as D5
Node solution->temperature Nearest Location   0.40  -6.03  -0.762  as D6
Node solution->temperature Nearest Location   0.40  -6.95  -0.762  as D7
Node solution->temperature Nearest Location   0.76  -1.08  -0.762  as E1
Node solution->temperature Nearest Location   0.76  -2.38  -0.762  as E2
Node solution->temperature Nearest Location   0.76  -3.29  -0.762  as E3
Node solution->temperature Nearest Location   0.76  -4.20  -0.762  as E4
Node solution->temperature Nearest Location   0.76  -5.12  -0.762  as E5
Node solution->temperature Nearest Location   0.76  -6.03  -0.762  as E6
Node solution->temperature Nearest Location   0.76  -6.95  -0.762  as E7
Node solution->temperature Nearest Location   1.13  -1.08  -0.762  as F1
Node solution->temperature Nearest Location   1.31  -1.51  -0.762  as F2
Node solution->temperature Nearest Location   1.49  -1.93  -0.762  as F3
Node solution->temperature Nearest Location   1.83  -2.76  -0.762  as F4
Node solution->temperature Nearest Location   3.01  -5.59  -0.762  as F5
Node solution->temperature Nearest Location   4.63  -9.52  -0.762  as F6
Node solution->temperature Nearest Location   6.98  -15.16 -0.762  as F7
Node solution->temperature Nearest Location   2.75  -1.08  -0.762  as G1
Node solution->temperature Nearest Location   3.09  -1.42  -0.762  as G2
Node solution->temperature Nearest Location   3.39  -1.72  -0.762  as G3
Node solution->temperature Nearest Location   4.03  -2.36  -0.762  as G4
Node solution->temperature Nearest Location   6.19  -4.52  -0.762  as G5
Node solution->temperature Nearest Location   9.21  -7.54  -0.762  as G6
Node solution->temperature Nearest Location  13.54 -11.87  -0.762  as G7
Node solution->temperature Nearest Location  2.75  -0.62  -0.762  as H1

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Node solution -> temperature Nearest Location  3.21  -0.62  -0.762  as H2
Node solution -> temperature Nearest Location  3.66  -0.62  -0.762  as H3
Node solution -> temperature Nearest Location  4.58  -0.62  -0.762  as H4
Node solution -> temperature Nearest Location  7.63  -0.62  -0.762  as H5
Node solution -> temperature Nearest Location 11.89  -0.62  -0.762  as H6
Node solution -> temperature Nearest Location 17.99  -0.62  -0.762  as H7
Node solution -> temperature Nearest Location  2.75  1.67  -0.762  as I1
Node solution -> temperature Nearest Location  3.21  1.67  -0.762  as I2
Node solution -> temperature Nearest Location  3.66  1.67  -0.762  as I3
Node solution -> temperature Nearest Location  4.58  1.67  -0.762  as I4
Node solution -> temperature Nearest Location  7.63  1.67  -0.762  as I5
Node solution -> temperature Nearest Location 11.89  1.67  -0.762  as I6
Node solution -> temperature Nearest Location 17.99  1.67  -0.762  as I7
Node solution -> temperature Nearest Location  2.75  3.96  -0.762  as J1
Node solution -> temperature Nearest Location  3.21  3.96  -0.762  as J2
Node solution -> temperature Nearest Location  3.66  3.96  -0.762  as J3
Node solution -> temperature Nearest Location  4.58  3.96  -0.762  as J4
Node solution -> temperature Nearest Location  7.63  3.96  -0.762  as J5
Node solution -> temperature Nearest Location 11.89  3.96  -0.762  as J6
Node solution -> temperature Nearest Location 17.99  3.96  -0.762  as J7
Node solution -> temperature Nearest Location  2.75  4.42  -0.762  as K1
Node solution -> temperature Nearest Location  3.09  4.76  -0.762  as K2
Node solution -> temperature Nearest Location  3.39  5.06  -0.762  as K3
Node solution -> temperature Nearest Location  4.03  5.70  -0.762  as K4
Node solution -> temperature Nearest Location  6.19  7.86  -0.762  as K5
Node solution -> temperature Nearest Location  9.21 10.88  -0.762  as K6
Node solution -> temperature Nearest Location 13.54 15.21  -0.762  as K7
Node solution -> temperature Nearest Location  0.00  4.42  -0.762  as L1
Node solution -> temperature Nearest Location  0.00  4.88  -0.762  as L2
Node solution -> temperature Nearest Location  0.00  5.33  -0.762  as L3
Node solution -> temperature Nearest Location  0.00  6.25  -0.762  as L4
Node solution -> temperature Nearest Location  0.00  9.30  -0.762  as L5
Node solution -> temperature Nearest Location  0.00 13.56  -0.762  as L6
Node solution -> temperature Nearest Location  0.00 15.21  -0.762  as L7
Node solution -> temperature Nearest Location  0.00  5.02  -0.762  as AB6
Node solution -> temperature Nearest Location  0.00  5.32  -0.762  as AB5
Node solution -> temperature Nearest Location  0.00  6.22  -0.762  as AB4
Node solution -> temperature Nearest Location  0.00  9.32  -0.762  as AB3
Node solution -> temperature Nearest Location  0.00 13.62  -0.762  as AB2
Node solution -> temperature Nearest Location  0.00 19.72  -0.762  as AB1
Node solution -> temperature Nearest Location  0.00 -1.68  -0.762  as BE6
Node solution -> temperature Nearest Location  0.00 -1.98  -0.762  as BE5
Node solution -> temperature Nearest Location  0.00 -2.88  -0.762  as BE4
Node solution -> temperature Nearest Location  0.00 -5.98  -0.762  as BE3
Node solution -> temperature Nearest Location  0.00 -10.28 -0.762  as BE2
Node solution -> temperature Nearest Location  0.00 -16.38 -0.762  as BE1

End History Output history_output_Aria

End Aria Region AriaRegion

BEGIN Adagio Region AdagioRegion

Use Finite Element Model adagio_FEM

Begin adaptive time stepping Adagio_ATS
    target iterations = 500
    method = material # <solver> | material
    cutback factor = 0.5 # <0.5>

END Adagio Region AdagioRegion

End History Output history_output_Aria

End Aria Region AriaRegion
growth factor = 1.05  # <1.5>
minimum multiplier = 0.0001
maximum multiplier = 1e+14
maximum failure cutbacks = 10  # <5>
iteration window = 5  # <target_iterations/10>
End adaptive time stepping Adagio_ATS

Begin solver Adagio_solver

Level 1 Predictor = default  # none | <default>

Begin Control Contact Adagio_Control_Contact

Level = 1
Target Relative Residual = 0.005
Acceptable Relative Residual = 100
Minimum Iterations = 1
Maximum Iterations = 1000
Reference = EXTERNAL  # <EXTERNAL> | INTERNAL

| BELYTSCHKO | RESIDUAL | ENERGY

End Control Contact Adagio_Control_Contact

Begin loadstep predictor Adagio_Loadstep_Predictor
type = scale_factor
scale factor = 1.0 0.0
End loadstep predictor Adagio_Loadstep_Predictor

Begin cg Adagio.CG

Line Search Tangent
Target Relative Residual = 0.0005
Acceptable Relative Residual = 0.01
# Iteration Reset = 10  # <10000>
Iteration Print = 400
Minimum Iterations = 1
Maximum Iterations = 50000
Preconditioner = diagonal  # <elastic> | block_initial

| probe | schur | diagonal

Balance Probe = 1  # <0> | 1 | 2
Nodal Probe Factor = 1e-06  # <1.0e-06>
Beta Method = PolakRibierePlus  # <PolakRibiere>

End cg Adagio.CG

End solver Adagio_solver

#########################################################
########## ADAGIO CONTACT DEFINITIONS ##########
#########################################################

Begin Contact Definition Adagio_WIPP_Room_B_Clay_Seams

Enforcement = Frictional

Contact Surface surf_3000 contains surface_3000
Contact Surface surf_3001 contains surface_3001
Contact Surface surf_3002 contains surface_3002
Contact Surface surf_3003 contains surface_3003
Contact Surface surf_3004 contains surface_3004
Contact Surface surf_3005 contains surface_3005
Contact Surface surf_3006 contains surface_3006
Contact Surface surf_3007 contains surface_3007
Contact Surface surf_3008 contains surface_3008
Contact Surface surf_3009 contains surface_3009
Contact Surface surf_3010 contains surface_3010
Contact Surface surf_3011 contains surface_3011
Contact Surface surf_3012 contains surface_3012
Contact Surface surf_3013 contains surface_3013
Contact Surface surf_3014 contains surface_3014
Contact Surface surf_3015 contains surface_3015
Contact Surface surf_3016 contains surface_3016
Contact Surface surf_3017 contains surface_3017

Begin Interaction Clay_D
    Master = surf_3000
    Slave = surf_3001
        Normal Tolerance = 0.01
        Tangential Tolerance = 0.1
        Capture Tolerance = 0.01
        Tension Release = 1e+20
        Friction Coefficient = 0.2
    End Interaction Clay_D

Begin Interaction Clay_E
    Master = surf_3002
    Slave = surf_3003
        Normal Tolerance = 0.01
        Tangential Tolerance = 0.1
        Capture Tolerance = 0.01
        Tension Release = 1e+20
        Friction Coefficient = 0.2
    End Interaction Clay_E

Begin Interaction Clay_F
    Master = surf_3004
    Slave = surf_3005
        Normal Tolerance = 0.01
        Tangential Tolerance = 0.1
        Capture Tolerance = 0.01
        Tension Release = 1e+20
        Friction Coefficient = 0.2
    End Interaction Clay_F

Begin Interaction Clay_G
    Master = surf_3006
    Slave = surf_3007
        Normal Tolerance = 0.01
        Tangential Tolerance = 0.1
        Capture Tolerance = 0.01
        Tension Release = 1e+20
        Friction Coefficient = 0.2
    End Interaction Clay_G

Begin Interaction Clay_H
    Master = surf_3008
    Slave = surf_3009
        Normal Tolerance = 0.01
        Tangential Tolerance = 0.1
        Capture Tolerance = 0.01
        Tension Release = 1e+20
        Friction Coefficient = 0.2
    End Interaction Clay_H

Begin Interaction Clay_I
    Master = surf_3010
    Slave = surf_3011
        Normal Tolerance = 0.01
        Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2

End Interaction Clay_I

Begin Interaction Clay_J
Master = surf_3012
Slave = surf_3013
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2

End Interaction Clay_J

Begin Interaction Clay_K
Master = surf_3014
Slave = surf_3015
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2

End Interaction Clay_K

Begin Interaction Clay_L
Master = surf_3016
Slave = surf_3017
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2

End Interaction Clay_L

End Contact Definition Adagio_WIPP_Room_B_Clay_Seams
Element Variables = stress as sig
Element Variables = unrotated_stress as usig
Element Variables = von_mises as vonmises
Element Variables = hydrostatic_stress as pressure
Element Variables = stress_invariant_1 as sinv1
Element Variables = stress_invariant_2 as sinv2
Element Variables = stress_invariant_3 as sinv3
Element Variables = max_principal_stress as psigm1
Element Variables = intermediate_principal_stress as psigm2
Element Variables = min_principal_stress as psigm3
Element Variables = max_shear_stress
Element Variables = octahedral_shear_stress as octahedral
Element Variables = temperature as temp
Element Variables = log_strain as strain
Element Variables = log_strain_invariant_1 as volstrain

End Results Output adagio_output

########################################################################
##### ADAGIO SIMULATION HISTORY RESULTS ######
########################################################################

Begin History Output adagio_history
  Database Name = roomb.h
  Database Type = exodusII
  At Time 0 Increment = 600 # Every 10.0 minutes
  At Time 3600 Increment = 3600 # Every hour
  At Time 86400 Increment = 86400 # Every day
  At Time 604800 Increment = 604800 # Every Week
  At Time 2629743.84 Increment = 2629743.84 # Every Month
  At Time 15778463.04 Increment = 1314871.92 # Every 0.5*months
  # At Time 2629743.84 Increment = 2629743.84 # Every Month
  At Time 15778463.04 Increment = 7889231.52 # Every 0.25*year
  Node displacement Nearest Location 0.0  -1.08 0 as A1
  Node displacement Nearest Location 0.0  -1.54 0 as A2
  Node displacement Nearest Location 0.0  -1.99 0 as A3
  Node displacement Nearest Location 0.0  -2.38 0 as A4
  Node displacement Nearest Location 0.0  -2.91 0 as A5
  Node displacement Nearest Location 0.0  -3.29 0 as A6
  Node displacement Nearest Location 0.0  -4.20 0 as A7
  Node displacement Nearest Location 0.0  -5.12 0 as A8
  Node displacement Nearest Location 0.0  -5.96 0 as A9
  Node displacement Nearest Location 0.0  -6.03 0 as A10
  Node displacement Nearest Location 0.0  -6.95 0 as A11
  Node displacement Nearest Location 0.0  -10.22 0 as A12
  Node displacement Nearest Location 0.0  -16.32 0 as A13
  Node displacement Nearest Location 2.75  -1.08 0 as G1
  Node displacement Nearest Location 3.09  -1.42 0 as G2
  Node displacement Nearest Location 3.39  -1.72 0 as G3
  Node displacement Nearest Location 4.03  -2.36 0 as G4
  Node displacement Nearest Location 6.19  -4.52 0 as G5
  Node displacement Nearest Location 9.21  -7.54 0 as G6
  Node displacement Nearest Location 13.54  -11.87 0 as G7
  Node displacement Nearest Location 2.75  1.67 0 as I1
  Node displacement Nearest Location 3.21  1.67 0 as I2
  Node displacement Nearest Location 3.66  1.67 0 as I3
  Node displacement Nearest Location 4.58  1.67 0 as I4
  Node displacement Nearest Location 7.63  1.67 0 as I5
  Node displacement Nearest Location 11.89  1.67 0 as I6
  Node displacement Nearest Location 17.99  1.67 0 as I7
  Node displacement Nearest Location 2.75  4.42 0 as K1
  Node displacement Nearest Location 3.09  4.76 0 as K2

End History Output adagio_history
Node displacement Nearest Location 3.39 5.06 0 as K3
Node displacement Nearest Location 4.03 5.70 0 as K4
Node displacement Nearest Location 6.19 7.86 0 as K5
Node displacement Nearest Location 9.21 10.88 0 as K6
Node displacement Nearest Location 13.54 15.21 0 as K7
Node displacement Nearest Location 0.00 4.88 0 as L2
Node displacement Nearest Location 0.00 5.33 0 as L3
Node displacement Nearest Location 0.00 6.25 0 as L4
Node displacement Nearest Location 0.00 9.30 0 as L5
Node displacement Nearest Location 0.00 13.56 0 as L6
Node displacement Nearest Location 0.00 15.21 0 as L7
Node displacement Nearest Location 2.75 0.30 0 as M1
Node displacement Nearest Location 3.66 0.30 0 as M2
Node displacement Nearest Location 4.58 0.30 0 as M3
Node displacement Nearest Location 7.63 0.30 0 as M4
Node displacement Nearest Location 11.89 0.30 0 as M5
Node displacement Nearest Location 17.99 0.30 0 as M6
Node displacement Nearest Location 2.75 -0.78 0 as N1
Node displacement Nearest Location 3.66 -0.78 0 as N2
Node displacement Nearest Location 2.75 4.12 0 as O1
Node displacement Nearest Location 17.99 4.12 0 as O2
Element stress Nearest Location 0.00 -1.08 -0.14 as P1
Element stress Nearest Location 0.00 -4.73 -0.14 as P2
Element stress Nearest Location 0.46 -1.08 -0.14 as Q1
Element stress Nearest Location 0.46 -8.69 -0.14 as Q2
Element stress Nearest Location 0.46 -16.32 -0.14 as Q3
Element stress Nearest Location 2.75 1.21 -0.14 as R1
Element stress Nearest Location 10.36 1.21 -0.14 as R2
Element stress Nearest Location 17.99 1.21 -0.14 as R3
Element stress Nearest Location 2.75 1.67 -0.14 as S1
Element stress Nearest Location 6.40 1.67 -0.14 as S2
Element stress Nearest Location 9.14 1.67 -0.14 as S3
Element stress Nearest Location 13.11 1.67 -0.14 as S4
Element stress Nearest Location 24.08 1.67 -0.14 as S5
Element stress Nearest Location 10.36 2.13 -0.14 as T1
Element stress Nearest Location 2.75 2.13 -0.14 as T2
Element stress Nearest Location 17.99 2.13 -0.14 as T3
Element stress Nearest Location 0.46 4.42 -0.14 as U1
Element stress Nearest Location 0.46 12.03 -0.14 as U2
Element stress Nearest Location 0.46 19.66 -0.14 as U3
Element stress Nearest Location 0.00 4.42 -0.14 as V1
Element stress Nearest Location 0.00 8.07 -0.14 as V2
End History Output adagio_history

#########################################################################
####### MECHANICAL INITIAL CONDITIONS #######
#########################################################################

Begin Initial Condition initialize_temperatureTemp
Include All Blocks
Initialize Variable Name = Temperature
Variable Type = Node
Magnitude = 300
End Initial Condition initialize_temperatureTemp

# Hydrostatic pressure initial condition (varies according to y-direction)
Begin initial condition initialize_stress_state
Initialize variable name = unrotated_stress
Variable type = element
Include All Blocks
Element Block Subroutine = geo_is
Subroutine Real Parameter: bot = -54.19
Subroutine Real Parameter: top = 52.87
Subroutine Real Parameter: po = -15980670.02
Subroutine Real Parameter: pl = -13570000
Subroutine Real Parameter: kvert_xx = 1
Subroutine Real Parameter: kvert_yy = 1
Subroutine Real Parameter: kvert_zz = 1
Subroutine Real Parameter: kvert_xy = 0
Subroutine Real Parameter: kvert_yz = 0
Subroutine Real Parameter: kvert_zx = 0
Subroutine String Parameter: dir = Y
End initial condition initialize_stress_state

Begin gravity Adagio_gravity
    Include all blocks
    Direction = y
    Gravitational constant = 9.79
    Scale Factor = -1.0
    Function = gravitational_acceleration_function
End gravity Adagio_gravity

#################################################
####### MECHANICAL BOUNDARY CONDITIONS ##########
#################################################
# 0 <= x <= 50 m; y=52.87 m
# Lithostatic pressure condition along top-side mesh (surface ID=2001)
Begin pressure
    Surface = surface_2001
    Scale Factor = 1.0
    Function = lithostatic_pressure_ytop_function
End pressure

# 0 <= x <= 50 m; y=-54.19 m
# Lithostatic pressure condition along bottom-side mesh (surface ID=2000)
Begin pressure
    Surface = surface_2000
    Scale Factor = 1.0
    Function = lithostatic_pressure_ybot_function
End pressure

# x=50 m; 49.38 m <= y <= +52.87 m; no xy-displacement; Anhydrite 7
# Fixed displacement condition along right-side mesh
Begin fixed displacement
    Components = x y
    Node Set = nodelist_101
End fixed displacement

# x=0 symmetry; no x-displacement
# Fixed x-displacement condition along left-side mesh
Begin fixed displacement
    Components = x
    Node Set = nodelist_100
End fixed displacement

# x=50 m; -54.19 m <= y 49.38 m; no x-displacement
# Fixed x-displacement condition along right-side mesh
Begin fixed displacement
    Components = x
    Node Set = nodelist_102
End fixed displacement

# z=0.0 m; 2D plane strain condition; no z-displacement
# Fixed z-displacement condition along z-bottom mesh
Begin fixed displacement
  Components = z
  Node Set = nodelist_400
End fixed displacement

# z=-0.28 m; 2D plane strain condition; no z-displacement
# Fixed z-displacement condition along z-top mesh
Begin fixed displacement
  Components = z
  Node Set = nodelist_401
End fixed displacement

End Adagio Region AdagioRegion

End Procedure arpeggio_procedure

END SIERRA WIPP_Room_B_Thermal_Structural_Funded_By_UFD
APPENDIX F: SIERRA MECHANICS OPERATORS USED IN THE HEATED ROOM COUPLED CALCULATION USING THE ENCLOSURE RADIATION METHOD

The SIERRA Mechanics transfer operators were similar of that described in Appendix D, except that there was no material ID #2 (i.e., block identifier 2 did not exist). The thermal mesh used in this calculation, using the radiation enclosure model, is shown in Figure 5-5. The structural mesh used in this calculation was identical as what was described in Section 5.1, and shown in Figure 4-12. Several coupled calculations were also conducted to investigate the sensitivity of normal flux directions involving the radiation enclosure definitions to provide insight on predicted temperature field influence. The normal flux directions were adjusted using the Cubit (Cubit, 2012) mesh tool, using the command language commands (and are related to the numerical mesh sideset Ids):

Sideset 4001 surface 4000 with respect to volume 1
Sideset 4002 surface 4002 with respect to volume 1
Sideset 4003 surface 4003 with respect to volume 1

This command sequence allowed the normal direction variable, internal to the mesh file, to be changed to a value of -1 or +1. The influence of the altering these normal flux directions had virtually no bearing on the computed temperature field, and the baseline and final normal flux directions, used in all of the coupled heated room calculations using the radiation enclosure method, are shown in Figure F-1.
Figure F-1 Enclosure Radiation Model Surface Normal Planes
# directory : /scratch/jsrath/NEAMS/roomb/coupled/simu001
# file : arpeggio.i
# author : Jonathan Scott Rath
# description : UFD 2012 WIPP Room B input deck
# UFD = Used Fuels Disposition
# WIPP = Waste Isolation Pilot Plant = WIPP
# SIERRA = Sandia Integrated Environment for Robust
# Research Algorithms
# SIERRA Thermal-Mechanical (Aria-Adagio) Calculation
# SIERRA TM WIPP Room B Two-Way Coupled Calculation
# Model 3 (Room B, Thermal+Mechanical)
# revision_log : 09/MARCH/2012
# - Modified time stepping for Adagio and Aria region
# : 01/MARCH/2012
# - Implemented new Sam Subia advised Enclosure
#  Radiation approach and method utilizing partial
#  enclosure constructs, etc.
# : 29/FEBRUARY/2012
# - Adapted new syntax for THERMAL STRAIN X FUNCTION
# - Adapted new syntax for THERMAL STRAIN Y FUNCTION
# - Adapted new syntax for THERMAL STRAIN Z FUNCTION
# - Using THERMAL LOG STRAIN X FUNCTION
# - Using THERMAL LOG STRAIN Y FUNCTION
# - Using THERMAL LOG STRAIN Z FUNCTION
# - Adapted heat flux at Room B opening to account
#  for normal outward direction
# - Added convection heat transfer boundary condition
# (Side Set 4000, h=0.51 W/m^2/K)
# - Added 3dHex8_MESH & 3dHex27_MESH variable control
# - Added non-conditional function tpf.include
# - Added non-conditional function ntc.include
# - Added coefficient of thermal expansion
# - Added power law thermal conductivity form
# - First Edition for "TM"
# unit system : System International (SI)
# mass = kilogram (kg)
# length = meter (m)
# time = seconds (sec)
# Temperature = Kelvin
# density = kg/(m^3)
# velocity = meter/sec = 10^-3*km/sec
# acceleration = m/(sec^2)
# force = mass * acceleration = kg*m/sec^2
# pressure = Newton / (m^2)
# = Pascal
# energy = Newton*m
# = Joule
# power = Joule/sec
# = Newton*m/sec
# = Watt

BEGIN SIERRA WIPP_Room_B_Thermal_Structural_Funded_By_UFD

Begin diagnostic control Adagio_Diagnostics
enable "tangent"
End diagnostic control Adagio_Diagnostics
define direction x with vector 1.0 0.0 0.0
define direction y with vector 0.0 1.0 0.0
define direction z with vector 0.0 0.0 1.0
define direction dir_1 with vector 0.7071067812 0.0 0.7071067812
define direction dir_2 with vector -0.7071067812 0.0 -0.7071067812
define point origin with coordinates 0.0 0.0 0.0

#define GLOBAL CONSTANTS

Begin Global Constants
Stefan Boltzmann Constant = 5.67e-08 \ (\text{watt (Nm/s)}/(\text{meter}^2*\text{degK}^4)}
End

#define FUNCTION DEFINITIONS

Begin definition for function DHLW_power_flux_function
Abscissa = time \ [# \ \text{[second]}]
Ordinate = DHLW_power_flux \ [# \ \text{(watt (Nm/s))}/(\text{meter}^2)]
Type = analytic
Evaluate Expression = "x <= 28080000 \ ? 0.0 : 228.012039*exp(-7.327e-10*x);"
Differentiate Expression is "x <= 28080000 \ ? 0.0 : -1.67064421e-07*exp(-7.327e-10*x);"
End definition for function DHLW_power_flux_function

Begin definition for function gravitational_acceleration_function
Type is piecewise linear
Begin values
0 1
157784630.4 1
End values
End definition for function gravitational_acceleration_function

Begin definition for function lithostatic_pressure_ybot_function
Type is piecewise linear
Begin values
0 15980670.02
157784630.4 15980670.02
End values
End definition for function lithostatic_pressure_ybot_function

Begin definition for function lithostatic_pressure_ytop_function
Type is piecewise linear
Begin values
0 13570000
157784630.4 13570000
End values
End definition for function lithostatic_pressure_ytop_function

# T_ref = 300 \ [\text{Kelvin}]
# T_max = 1500 \ [\text{Kelvin}]
# alpha = 2.4e-05 \ [1/\text{Kelvin}]
# -----------------------------
# T_ref = 0.0
# T_max = (T_max-T_ref)*alpha
# -----------------------------
Begin definition for function polyhalite_thermal_strain_function
   Type is piecewise linear
   Begin values
   300 0
   1500 0.0288
   End values
End definition for function polyhalite_thermal_strain_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 4e-05 [1/Kelvin]
# ----------------------------
# T_ref    0.0
# T_max    (T_max-T_ref)*alpha
# ----------------------------

Begin definition for function argillaceous_thermal_strain_function
   Type is piecewise linear
   Begin values
   300 0
   1500 0.048
   End values
End definition for function argillaceous_thermal_strain_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 2e-05 [1/Kelvin]
# ----------------------------
# T_ref    0.0
# T_max    (T_max-T_ref)*alpha
# ----------------------------

Begin definition for function anhydrite_thermal_strain_function
   Type is piecewise linear
   Begin values
   300 0
   1500 0.024
   End values
End definition for function anhydrite_thermal_strain_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 4.5e-05 [1/Kelvin]
# ----------------------------
# T_ref    0.0
# T_max    (T_max-T_ref)*alpha
# ----------------------------

Begin definition for function halite_thermal_strain_function
   Type is piecewise linear
   Begin values
   300 0
   1500 0.054
   End values
End definition for function halite_thermal_strain_function

Begin definition for function polyhalite_pressure_volstrain_function
   Type is piecewise linear
   Ordinate is volumetric_strain
   Abscissa is Pressure
   Begin values
   -1 -6.583333333e+10 # -65833.33333 MPa
   0 0
   1 6.583333333e+10 # 65833.33333 MPa
   End values
End definition for function polyhalite_pressure_volstrain_function
Begin definition for function anhydrite_pressure_volstrain_function
  Type is piecewise linear
  Ordinate is volumetric_strain
  Abscissa is Pressure
  Begin values
  -1 -8.344444444e+10 # -83444.44444 MPa
  0 0
  1 8.344444444e+10 # 83444.44444 MPa
  End values
End definition for function anhydrite_pressure_volstrain_function

Begin Property Specification for material polyhalite
  Density = 2300
  thermal log strain x function = polyhalite_thermal_strain_function
  thermal log strain y function = polyhalite_thermal_strain_function
  thermal log strain z function = polyhalite_thermal_strain_function
  Begin parameters for model soil_foam
    Youngs modulus = 5.53e+10 # [Pa]
    Poissons ratio = 0.36 # [dimensionless]
    #    Bulk modulus = 6.583333333e10 # [Pa]
    #    Shear modulus = 2.033088235e+10 # [Pa]
    a0 = 2459512.147 # [Pa]
    a1 = 2.457780096
    a2 = 0 # [1/Pa]
    pressure cutoff = -1000704.722 # [Pa]
    pressure function = polyhalite_pressure_volstrain_function
  End parameters for model soil_foam
End Property Specification for material polyhalite

Begin Property Specification for material argillaceous
  Density = 2300
  thermal log strain x function = argillaceous_thermal_strain_function
  thermal log strain y function = argillaceous_thermal_strain_function
  thermal log strain z function = argillaceous_thermal_strain_function
  Begin Parameters For Model MD_Creep
    #            Youngs Modulus = 3.100000833e+10
    #            Poissons Ratio = 0.250000336
    #    Lambda = 1.240003333e10
    #    Two Mu = 2.48e+10
    Bulk Modulus = 2.06667e+10
    Shear Modulus = 1.24e+10
    A1 = 1.406e+23
    Q1/R = 12581.78
    #    Q1/RT = 41.93926667 # Isothermal, T=300 Kelvin
    N1 = 5.5
    B1 = 8993300
    A2 = 1.3131e+13
    Q2/R = 5032.71
    #    Q2/RT = 16.7757 # Isothermal, T=300 Kelvin
End Parameters For Model MD_Creep

N2 = 5
B2 = 0.042875
Sig0 = 20570000
Qlc = 5335
M = 3
K0 = 2470000
# CSTAR = 0.009189
# TK = 300
# C = 2.759 # C = CSTAR/TK (MD Creep model uses C when isothermal)
C = 0.009189 # C (MD Creep model uses C=CSTAR when nonisothermal)
Alpha = -14.96
Beta = -7.738
Deltalc = 0.58
Amult = 0.5
Grwfac = 1.05
Epstol = 0.005
Shkfac = 1
Itype = 0
Angle = 0.1

End Parameters For Model MD_Creep

End Property Specification for material argillaceous

Begin Property Specification for material anhydrite
Density = 2300
thermal log strain x function = anhydrite_thermal_strain_function
thermal log strain y function = anhydrite_thermal_strain_function
thermal log strain z function = anhydrite_thermal_strain_function

Begin parameters for model soil_foam
youngs modulus = 7.51e+10 # [Pa]
poissons ratio = 0.35 # [dimensionless]
bulk modulus = 8.344444444e+10 # [Pa]
shear modulus = 2.781481481e+10 # [Pa]
a0 = 2338268.59 # [Pa]
a1 = 2.33826859
a2 = 0 # [1/Pa]
pressure cutoff = -1000000 # [Pa]
pressure function = anhydrite_pressure_volstrain_function

End Parameters for model soil_foam

End Property Specification for material anhydrite

Begin Property Specification for material halite
Density = 2300
thermal log strain x function = halite_thermal_strain_function
thermal log strain y function = halite_thermal_strain_function
thermal log strain z function = halite_thermal_strain_function

Begin Parameters For Model MD_Creep
# Youngs Modulus = 3.1e+10
# Poissons Ratio = 0.25
# Lambda = 1.24e+10
# Two Mu = 2.48e+10

Bulk Modulus = 2.066666667e+10
Shear Modulus = 1.24e+10
A1 = 8.386e+22
Q1/R = 12581.78158

Q1/RT = 41.93927193 # Isothermal, T=300 Kelvin
N1 = 5.5
B1 = 6086000
A2 = 9.672e+12
Q2/R = 5032.712632

Q2/RT = 16.77570877 # Isothermal, T=300 Kelvin
N2 = 5
B2 = 0.03034
Sig0 = 20570000
Qlc = 5335
M = 3
X0 = 627500
# CSTAR = 0.009189
# TK = 300
# C = 2.759 # C = CSTAR/TK (MD Creep model uses C when isothermal)
# C = 0.009189 # C (MD Creep model uses C=CSTAR when nonisothermal)
Alpha = -17.37
Beta = -7.738
Deltalc = 0.58
Amult = 0.5
Grwfac = 1.05
Epstol = 0.005
Shkfac = 1
Itype = 0
Angle = 0.1
End Parameters For Model MD_Creep
End Property Specification for material halite

Begin Aria Material ONE
Density = Constant Rho = 2300 # [kg/m^3]
Thermal Conductivity = Power_law A = 3333.406168 gamma = -1.14
Specific heat = Constant Cp = 860 # [joule (Nm)]/(kilogram*degK)
Emissivity = Constant e = 0.8 # [1]
Heat Conduction = basic
End Aria Material ONE

# Material TWO (previously known as "thermal equivalent material")
# Not used in coupled thermal-structural calculation (arpeggio).
# Begin Aria material TWO
# Density = Constant Rho = 1 # [kg/m^3]
# Thermal Conductivity = Constant K = 50 # [watt (Nm/s)]/(meter*degK)
# Specific heat = Constant Cp = 1000 # [joule (Nm)]/(kilogram*degK)
# Emissivity = Constant e = 0.3 # [1]
# Heat Conduction = basic
# End Aria material TWO
#

### FINITE ELEMENT MODELS

Begin Finite Element Model Adagio_FEM
Database Name = roomb.g
Database Type = exodusII

Begin parameters for block block_1
material polyhalite
solid mechanics use model soil_foam
section = hex8
hourglass stiffness = 0.003
End Parameters for block block_1

Begin parameters for block block_2
material argillaceous
solid mechanics use model MD_Creep
section = hex8
hourglass stiffness = 0.003
End Parameters for block block_2

Begin parameters for block block_3
material anhydrite
solid mechanics use model soil_foam
section = hex8
hourglass stiffness = 0.003
End Parameters for block block_3

Begin parameters for block block_4
material halite
solid mechanics use model MD_Creep
section = hex8
hourglass stiffness = 0.003
End Parameters for block block_4

End Finite Element Model Adagio_FEM

Begin Finite Element Model Aria_FEM

Database Name = roombq.g
Database Type = exodusII
Coordinate System is cartesian

Use Material ONE for block_1
#
# Material TWO not used in coupled thermal-structural calculation (arpeggio).
# (previously known as "thermal equivalent material")
#
# Omit Volume block_2
# Use Material TWO for block_2
#

End Finite Element Model Aria_FEM

####################################################################
################# LINEAR SOLVERS ###################################
####################################################################

Begin Aztec Equation Solver AriaLinearEquationSolverAztec
  Solution Method = cg
  Preconditioning Method = DD-ICC
  Maximum Iterations = 500
  Residual Norm Tolerance = 1e-08
  Residual Norm Scaling = r0
End Aztec Equation Solver AriaLinearEquationSolverAztec

Begin Trilinos Equation Solver AriaLinearEquationSolverTrilinos
  Solution Method = cg
  Preconditioning Method = multilevel #jacobi
  Maximum Iterations = 2000
  Residual Norm Scaling = r0
  Residual Norm Tolerance = 1.0e-08
End Trilinos Equation Solver AriaLinearEquationSolverTrilinos

####################################################################
################ ARPEGGIO PROCEDURE ################################
####################################################################

Begin Procedure arpeggio_procedure
Begin Solution Control Description
Use System Main

Begin System Main
Simulation Start Time = 0
Simulation Termination Time = 157784630.4 # 5 [years] = 1826.211 [days]
Simulation Max Global Iterations = 1e+12
Begin Transient Time_Block_1
Advance AriaRegion
Transfer Aria_to_Adagio
Advance AdagioRegion
Transfer Adagio_to_Aria
End Transient Time_Block_1
Begin Transient Time_Block_2
Advance AriaRegion
Transfer Aria_to_Adagio
Advance AdagioRegion
Transfer Adagio_to_Aria
End Transient Time_Block_2
End System Main

Begin Parameters For Transient Time_Block_1
Start Time = 0
Termination Time = 28080000 # 0.8898205081 [years] = 325 [days]
Begin Parameters For Aria Region AriaRegion
Time Integration Method = Second_Order
Time Step Variation = Adaptive
Initial Time Step Size = 1e-06
Minimum Time step Size = 5e-07
Maximum Time step Size = 26055 # 0.00082565076 [years] = 0.3015625 [days]
Maximum Time Step Size ratio = 10
Minimum Resolved Time Step Size = 5e-07
Predictor-Corrector Tolerance = 0.0005
Predictor-Corrector Normalization = MAX
End Parameters for Aria Region AriaRegion
Begin parameters for Adagio Region AdagioRegion
Time Increment = 1e-06
End Parameters for Adagio Region AdagioRegion
End Parameters for Transient Time_Block_1

Begin Parameters For Transient Time_Block_2
Start Time = 28080000 # 0.8898205081 [years] = 325 [days]
Termination Time = 157784630.4 # 5 [years] = 1826.211 [days]
Begin Parameters For Aria Region AriaRegion
Time Integration Method = Second_Order
Time Step Variation = Adaptive
Initial Time Step Size = 100 # 3.168876454e-06 [years] = 0.001157407407 [days]
Minimum Time step Size = 50
Maximum Time step Size = 864000 # 0.02737909256 [years] = 10 [days]
Maximum Time Step Size ratio = 10
Minimum Resolved Time Step Size = 50
Predictor-Corrector Tolerance = 0.0005
Predictor-Corrector Normalization = MAX
End Parameters for Aria Region AriaRegion
Begin parameters for Adagio Region AdagioRegion
Time Increment = 100 # 3.168876454e-06 [years] = 0.001157407407 [days]
End Parameters for Adagio Region AdagioRegion
End Parameters For Transient Time_Block_2
End Solution Control Description

########################################################################
# SIERRA CODE TO CODE TRANSFERS
########################################################################

Begin Transfer Aria_to_Adagio
Interpolate Volume Nodes from AriaRegion to AdagioRegion
Send Field Solution->Temperature State New to Temperature State New
Search Coordinate Field model_coordinates state none to model_coordinates
Send Block block_1 to block_1 block_2 block_3 block_4
End Transfer Aria_to_Adagio

Begin Transfer Adagio_to_Aria
Interpolate Volume Nodes from AdagioRegion to AriaRegion
Send Field Displacement State New to Solution->Mesh_Displacements State New
Search Coordinate Field model_coordinates state none to model_coordinates
Send Block block_1 block_2 block_3 block_4 to block_1
End Transfer Adagio_to_Aria

########################################################################
# ARIA REGION
########################################################################

Begin Aria Region AriaRegion
Use Finite Element Model Aria_FEM
Use Linear Solver AriaLinearEquationSolverAztec
Nonlinear Solution Strategy = Newton
NONLINEAR RESIDUAL TOLERANCE = 1.0e-6
MAXIMUM NONLINEAR ITERATIONS = 5
NONLINEAR RELAXATION FACTOR = 1.0
Use DOF Averaged Nonlinear Residual
Accept Solution After Maximum Nonlinear Iterations = true

########################################################################
# GOVERNING EQUATIONS
########################################################################
# Energy for Temperature on All_blocks using Q1 with Lumped_Mass DIFF
# SRC
# Mesh for Mesh_Displacements on All_blocks using Q1 with Xfer
## (Only block_1 in FY2012 coupled thermal-structural simulations)
## Energy for Temperature on block_1 using Q1 with Lumped_Mass DIFF
## SRC
## Mesh for Mesh_Displacements on block_1 using Q1 with Xfer
## (No block_2, previously known as the "equivalent thermal material")
## Energy for Temperature on block_2 using Q1 with Lumped_Mass DIFF
## SRC
## Mesh for Mesh_Displacements on block_2 using Q1 with Xfer
PostProcess HEAT_FLUX on All_Blocks using Q1

########################################################################
# THERMAL INITIAL CONDITIONS
########################################################################
IC CONST on All_blocks Temperature = 300

################################################
########## THERMAL BOUNDARY CONDITIONS ##########
################################################
# Adiabatic or Isentropic BC (i.e., "von Neuman") energy flux = 0
# von Neuman B.C. left symmetry
BC Flux for Energy on surface_1000 = constant flux = 0.0
# von Neuman B.C. right far-field
BC Flux for Energy on surface_1001 = constant flux = 0.0
# von Neuman B.C. y-vertical bottom model
BC Flux for Energy on surface_2000 = constant flux = 0.0
# von Neuman B.C. y-vertical top model
BC Flux for Energy on surface_2001 = constant flux = 0.0

################################################
############# VIEWFACTOR DEFINITIONS ############
################################################
Begin Viewfactor Calculation VFC_YZ_PAIRWISE
  Compute Rule = pairwise
  Output Rule = summary
  y-z plane symmetry
End Viewfactor Calculation VFC_YZ_PAIRWISE

Begin Viewfactor Smoothing VFS1
  Method = least-squares
  Output Rule = summary
End Viewfactor Smoothing VFS1

Begin Radiosity Solver RS1
  Coupling = mason
  Solver = chaparral CG
  Convergence Tolerance = 1.0e-13
  Maximum Iterations = 1000
  Output Rule = summary
End Radiosity Solver RS1

################################################
############# ENCLOSURE DEFINITIONS ############
################################################
# Surface_4001 is Room B Floor (y=-1.08 m), normal_direction = -1
# Surface_4002 is Room B Pillar Right Side (x=2.75 m), normal_direction = 1
# Surface_4003 is Room B Roof (y=4.42 m), normal_direction = 1
Begin Enclosure Definition WIPP_ROOM_B
  Add surface surface_4001 surface_4002 surface_4003
  Use viewfactor calculation VFC_YZ_PAIRWISE
  Use viewfactor smoothing VFS1
  Use radiosity solver RS1
  Integrated power output encl_roombq_power
  Integrated flux output encl_roombq_flux
  Partial Enclosure Temperature = 300 # effective inifinte zpos and zneg temperature
  Partial Enclosure Emissivity = 1 # guess of emissivity
  Partial Enclosure Area = 30.25 # area of two sides bounding Room B drift opening (x-y plane)
Viewfactor Update is Interval Using 3155692.608
# Database Name is viewfactor/encl_WIPP_ROOM_B.vf in binary format
# Rowsum Database Name is viewfactor/encl_WIPP_ROOM_B_rowsum
End Enclosure Definition WIPP_ROOM_B

################################################
############## SURFACE HEAT SOURCE ##############
################################################
# BC Flux for Energy on surface_6666 = Function Name = DHLW_power_flux_function
Begin Heat Flux Boundary Condition Aria_DHLW
  Add Surface surface_6666
  Flux Time Function = DHLW_power_flux_function
End Heat Flux Boundary Condition Aria_DHLW

################################################
######## ARIA SIMULATION OUTPUT RESULTS ########
################################################
Begin Results Output output_Aria
  Database Name = roombq.e
  Database Type = ExodusII
  Global Variables = time_step as timestep
  Global Variables = encl_roombq_power
  Global Variables = encl_roombq_flux
  Nodal Variables = solution->mesh_displacements as displ
  Nodal Variables = solution->temperature as temp
  Nodal Variables = pp->HEAT_FLUX as heatflux
  Timestep Adjustment Interval = 4
  At time 0, Increment = 604800 # ( t=0 seconds, incr=1 weeks )
  At time 15778463.04, Increment = 2629743.84 # ( t=0.5 years, incr=1 months )
  At time 31556926.08, Increment = 2629743.84 # ( t=1 years, incr=1 months )
  At time 63113852.16, Increment = 2629743.84 # ( t=2 years, incr=1 months )
  At time 94670778.24, Increment = 2629743.84 # ( t=3 years, incr=1 months )
  At time 126227704.3, Increment = 2629743.84 # ( t=4 years, incr=1 months )
  At time 157784630.4, Increment = 2629743.84 # ( t=5 years, incr=1 months )
  Termination Time = 157784630.4 # 5 years
End Results Output output_Aria

################################################
####### ARIA SIMULATION HISTORY RESULTS ########
################################################
Begin History Output history_output_Aria
  Database Name = roombq.h
  Database Type = ExodusII
  At time 0, Increment = 604800 # ( t=0 seconds, incr=1 weeks )
  At time 15778463.04, Increment = 2629743.84 # ( t=0.5 years, incr=1 months )
  At time 31556926.08, Increment = 2629743.84 # ( t=1 years, incr=1 months )
  At time 63113852.16, Increment = 2629743.84 # ( t=2 years, incr=1 months )
  At time 94670778.24, Increment = 2629743.84 # ( t=3 years, incr=1 months )
  At time 126227704.3, Increment = 2629743.84 # ( t=4 years, incr=1 months )
  At time 157784630.4, Increment = 2629743.84 # ( t=5 years, incr=1 months )
  Termination Time = 157784630.4 # 5 years
End History Output history_output_Aria
Node solution->temperature Nearest Location  0.0  -5.12  -0.762  as A8
Node solution->temperature Nearest Location  0.0  -5.96  -0.762  as A9
Node solution->temperature Nearest Location  0.0  -6.03  -0.762  as A10
Node solution->temperature Nearest Location  0.0  -10.22  -0.762  as A12
Node solution->temperature Nearest Location  0.0  -16.32  -0.762  as A13
Node solution->temperature Nearest Location  0.15  -1.08  -0.762  as B1
Node solution->temperature Nearest Location  0.15  -3.37  -0.762  as B2
Node solution->temperature Nearest Location  0.15  -4.01  -0.762  as B3
Node solution->temperature Nearest Location  0.15  -4.65  -0.762  as B4
Node solution->temperature Nearest Location  0.15  -5.32  -0.762  as B5
Node solution->temperature Nearest Location  0.15  -5.96  -0.762  as B6
Node solution->temperature Nearest Location  0.21  -1.08  -0.762  as C1
Node solution->temperature Nearest Location  0.21  -2.38  -0.762  as C2
Node solution->temperature Nearest Location  0.21  -3.29  -0.762  as C3
Node solution->temperature Nearest Location  0.21  -4.20  -0.762  as C4
Node solution->temperature Nearest Location  0.40  -1.08  -0.762  as D1
Node solution->temperature Nearest Location  0.40  -2.38  -0.762  as D2
Node solution->temperature Nearest Location  0.40  -3.29  -0.762  as D3
Node solution->temperature Nearest Location  0.40  -4.20  -0.762  as D4
Node solution->temperature Nearest Location  0.40  -5.12  -0.762  as D5
Node solution->temperature Nearest Location  0.40  -6.03  -0.762  as D6
Node solution->temperature Nearest Location  0.40  -6.95  -0.762  as D7
Node solution->temperature Nearest Location  0.76  -1.08  -0.762  as E1
Node solution->temperature Nearest Location  0.76  -2.38  -0.762  as E2
Node solution->temperature Nearest Location  0.76  -3.29  -0.762  as E3
Node solution->temperature Nearest Location  0.76  -4.20  -0.762  as E4
Node solution->temperature Nearest Location  0.76  -5.12  -0.762  as E5
Node solution->temperature Nearest Location  0.76  -6.03  -0.762  as E6
Node solution->temperature Nearest Location  0.76  -6.95  -0.762  as E7
Node solution->temperature Nearest Location  1.13  -1.08  -0.762  as F1
Node solution->temperature Nearest Location  1.31  -1.51  -0.762  as F2
Node solution->temperature Nearest Location  1.49  -1.93  -0.762  as F3
Node solution->temperature Nearest Location  1.83  -2.76  -0.762  as F4
Node solution->temperature Nearest Location  3.01  -5.59  -0.762  as F5
Node solution->temperature Nearest Location  4.63  -9.52  -0.762  as F6
Node solution->temperature Nearest Location  6.98 -15.16  -0.762  as F7
Node solution->temperature Nearest Location  2.75  -1.08  -0.762  as G1
Node solution->temperature Nearest Location  3.09  -1.42  -0.762  as G2
Node solution->temperature Nearest Location  3.39  -1.72  -0.762  as G3
Node solution->temperature Nearest Location  4.03  -2.36  -0.762  as G4
Node solution->temperature Nearest Location  6.19  -4.52  -0.762  as G5
Node solution->temperature Nearest Location  9.21  -7.54  -0.762  as G6
Node solution->temperature Nearest Location  13.54 -11.87  -0.762  as G7
Node solution->temperature Nearest Location  2.75  -0.62  -0.762  as H1
Node solution->temperature Nearest Location  3.21  -0.62  -0.762  as H2
Node solution->temperature Nearest Location  3.66  -0.62  -0.762  as H3
Node solution->temperature Nearest Location  4.58  -0.62  -0.762  as H4
Node solution->temperature Nearest Location  7.63  -0.62  -0.762  as H5
Node solution->temperature Nearest Location  11.89  -0.62  -0.762  as H6
Node solution->temperature Nearest Location  17.99  -0.62  -0.762  as H7
Node solution->temperature Nearest Location  2.75  1.67  -0.762  as I1
Node solution->temperature Nearest Location  3.21  1.67  -0.762  as I2
Node solution->temperature Nearest Location  3.66  1.67  -0.762  as I3
Node solution->temperature Nearest Location  4.58  1.67  -0.762  as I4
Node solution->temperature Nearest Location  7.63  1.67  -0.762  as I5
Node solution->temperature Nearest Location  11.89  1.67  -0.762  as I6
Node solution->temperature Nearest Location  17.99  1.67  -0.762  as I7
Node solution->temperature Nearest Location  2.75  3.96  -0.762  as J1
Node solution->temperature Nearest Location  3.21  3.96  -0.762  as J2
<table>
<thead>
<tr>
<th>Node solution-&gt;temperature Nearest Location</th>
<th>Temperature</th>
<th>Relative Residual</th>
<th>Adagio</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.66</td>
<td>3.96</td>
<td>-0.762</td>
<td>J3</td>
<td></td>
</tr>
<tr>
<td>4.58</td>
<td>3.96</td>
<td>-0.762</td>
<td>J4</td>
<td></td>
</tr>
<tr>
<td>7.63</td>
<td>3.96</td>
<td>-0.762</td>
<td>J5</td>
<td></td>
</tr>
<tr>
<td>11.89</td>
<td>3.96</td>
<td>-0.762</td>
<td>J6</td>
<td></td>
</tr>
<tr>
<td>17.99</td>
<td>3.96</td>
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<td>J7</td>
<td></td>
</tr>
<tr>
<td>2.75</td>
<td>4.42</td>
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<td>K1</td>
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<td>4.76</td>
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<td>K2</td>
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</tr>
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<td>K3</td>
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<td>K6</td>
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<td>15.21</td>
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<td>L2</td>
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<td>L6</td>
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<td>L7</td>
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</tr>
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<td>-0.762</td>
<td>AB5</td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>6.22</td>
<td>-0.762</td>
<td>AB4</td>
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</tr>
<tr>
<td>0.00</td>
<td>9.32</td>
<td>-0.762</td>
<td>AB3</td>
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</tr>
<tr>
<td>0.00</td>
<td>13.62</td>
<td>-0.762</td>
<td>AB2</td>
<td></td>
</tr>
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<td>AB1</td>
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</tr>
<tr>
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<td>BE6</td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>-1.98</td>
<td>-0.762</td>
<td>BE5</td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>-2.88</td>
<td>-0.762</td>
<td>BE4</td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>-5.98</td>
<td>-0.762</td>
<td>BE3</td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>-10.28</td>
<td>-0.762</td>
<td>BE2</td>
<td></td>
</tr>
<tr>
<td>0.00</td>
<td>-16.38</td>
<td>-0.762</td>
<td>BE1</td>
<td></td>
</tr>
</tbody>
</table>
Minimum Iterations = 1
Maximum Iterations = 1000
Reference = EXTERNAL # <EXTERNAL> | INTERNAL

<table>
<thead>
<tr>
<th>BELYTSCHKO</th>
<th>RESIDUAL</th>
<th>ENERGY</th>
</tr>
</thead>
</table>
End Control Contact Adagio_Control_Contact

Begin loadstep predictor Adagio_Loadstep_Predictor
type = scale_factor
scale factor = 1.0 0.0
End loadstep predictor Adagio_Loadstep_Predictor

Begin cg Adagio_CG
Line Search Tangent
Target Relative Residual = 0.0005
Acceptable Relative Residual = 0.01
#
Iteration Reset = 10 # <10000>
Iteration Print = 400
Minimum Iterations = 1
Maximum Iterations = 50000
Preconditioner = diagonal # <elastic> | block_initial
Balance Probe = 1 # <0> | 1 | 2
Nodal Probe Factor = 1e-06 # <1.0e-06>
Beta Method = PolakRibierePlus # <PolakRibiere> |
PolakRibierePlus | FletcherReeves
End cg Adagio_CG

End solver Adagio_solver

#########################################################################
# ADAGIO CONTACT DEFINITIONS #
#########################################################################
Begin Contact Definition Adagio_WIPP_Room_B_Clave_Seams
Enforcement = Frictional

Contact Surface surf_3000 contains surface_3000
Contact Surface surf_3001 contains surface_3001
Contact Surface surf_3002 contains surface_3002
Contact Surface surf_3003 contains surface_3003
Contact Surface surf_3004 contains surface_3004
Contact Surface surf_3005 contains surface_3005
Contact Surface surf_3006 contains surface_3006
Contact Surface surf_3007 contains surface_3007
Contact Surface surf_3008 contains surface_3008
Contact Surface surf_3009 contains surface_3009
Contact Surface surf_3010 contains surface_3010
Contact Surface surf_3011 contains surface_3011
Contact Surface surf_3012 contains surface_3012
Contact Surface surf_3013 contains surface_3013
Contact Surface surf_3014 contains surface_3014
Contact Surface surf_3015 contains surface_3015
Contact Surface surf_3016 contains surface_3016
Contact Surface surf_3017 contains surface_3017

Begin Interaction Clay_D
Master = surf_3000
Slave = surf_3001
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_D

Begin Interaction Clay_E
Master = surf_3002
Slave = surf_3003
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_E

Begin Interaction Clay_F
Master = surf_3004
Slave = surf_3005
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_F

Begin Interaction Clay_G
Master = surf_3006
Slave = surf_3007
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_G

Begin Interaction Clay_H
Master = surf_3008
Slave = surf_3009
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_H

Begin Interaction Clay_I
Master = surf_3010
Slave = surf_3011
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_I

Begin Interaction Clay_J
Master = surf_3012
Slave = surf_3013
Normal Tolerance = 0.01
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_J
Begin Interaction Clay_K
  Master = surf_3014
  Slave = surf_3015
  Normal Tolerance = 0.01
  Tangential Tolerance = 0.1
  Capture Tolerance = 0.01
  Tension Release = 1e+20
  Friction Coefficient = 0.2
End Interaction Clay_K

Begin Interaction Clay_L
  Master = surf_3016
  Slave = surf_3017
  Normal Tolerance = 0.01
  Tangential Tolerance = 0.1
  Capture Tolerance = 0.01
  Tension Release = 1e+20
  Friction Coefficient = 0.2
End Interaction Clay_L

End Contact Definition Adagio_WIPP_Room_B_Clay_Seams

###############################################################################
####### ADAGIO SIMULATION OUTPUT RESULTS #########
###############################################################################

Begin Results Output adagio_output

Database Name = roomb.e
Database Type = exodusII

At Time 0 Increment = 600 # Every 10.0 minutes
At Time 3600 Increment = 3600 # Every hour
At Time 86400 Increment = 86400 # Every day
At Time 604800 Increment = 604800 # Every Week
At Time 2629743.84 Increment = 2629743.84 # Every Month
At Time 15778463.04 Increment = 7889231.52 # Every 0.5*Months
At Time 47335389.12 Increment = 7889231.52 # Every 0.25*year

Global Variables = timestep
Global Variables = kinetic_energy
Global Variables = contact_energy
Nodal Variables = velocity
Nodal Variables = displacement
Element Variables = stress
Element Variables = unrotated_stress
Element Variables = von_mises
Element Variables = hydrostatic_stress
Element Variables = stress_invariant_1
Element Variables = stress_invariant_2
Element Variables = stress_invariant_3
Element Variables = max_principal_stress
Element Variables = intermediate_principal_stress
Element Variables = min_principal_stress
Element Variables = max_shear_stress
Element Variables = octahedral_shear_stress
Element Variables = temperature
Element Variables = log_strain

150
Element Variables = log_strain_invariant_1 as volstrain

End Results Output adagio_output

#########################################################################
# ADAGIO SIMULATION HISTORY RESULTS #######
#########################################################################

Begin History Output adagio_history
Database Name = roomb.h
Database Type = exodusII
At Time 0 Increment = 600 # Every 10.0 minutes
At Time 3600 Increment = 3600 # Every hour
At Time 86400 Increment = 86400 # Every day
At Time 604800 Increment = 604800 # Every Week
At Time 2629743.84 Increment = 2629743.84 # Every Month
At Time 47335389.12 Increment = 7889231.52 # Every 0.25*year
# At Time 2629743.84 Increment = 2629743.84 # Every Month
# At Time 15778463.04 Increment = 7889231.52 # Every 0.25*year
Node displacement Nearest Location 0.0 -1.08 0 as A1
Node displacement Nearest Location 0.0 -1.54 0 as A2
Node displacement Nearest Location 0.0 -1.99 0 as A3
Node displacement Nearest Location 0.0 -2.38 0 as A4
Node displacement Nearest Location 0.0 -2.69 0 as A5
Node displacement Nearest Location 0.0 -3.29 0 as A6
Node displacement Nearest Location 0.0 -4.00 0 as A7
Node displacement Nearest Location 0.0 -4.44 0 as A8
Node displacement Nearest Location 0.0 -5.96 0 as A9
Node displacement Nearest Location 0.0 -6.03 0 as A10
Node displacement Nearest Location 0.0 -6.95 0 as A11
Node displacement Nearest Location 0.0 -10.22 0 as A12
Node displacement Nearest Location 0.0 -16.32 0 as A13
Node displacement Nearest Location 2.75 -1.08 0 as G1
Node displacement Nearest Location 3.09 -1.42 0 as G2
Node displacement Nearest Location 3.39 -1.72 0 as G3
Node displacement Nearest Location 3.39 -1.72 0 as G3
Node displacement Nearest Location 3.39 -1.72 0 as G3
Node displacement Nearest Location 3.39 -1.72 0 as G3
Node displacement Nearest Location 3.39 -1.72 0 as G3
Node displacement Nearest Location 3.39 -1.72 0 as G3
Node displacement Nearest Location 3.39 -1.72 0 as G3
Node displacement Nearest Location 4.03 -2.36 0 as G4
Node displacement Nearest Location 6.19 -4.52 0 as G5
Node displacement Nearest Location 9.21 -7.54 0 as G6
Node displacement Nearest Location 13.54 -11.87 0 as G7
Node displacement Nearest Location 2.75 1.67 0 as I1
Node displacement Nearest Location 3.21 1.67 0 as I2
Node displacement Nearest Location 3.66 1.67 0 as I3
Node displacement Nearest Location 4.58 1.67 0 as I4
Node displacement Nearest Location 7.63 1.67 0 as I5
Node displacement Nearest Location 11.89 1.67 0 as I6
Node displacement Nearest Location 17.99 1.67 0 as I7
Node displacement Nearest Location 2.75 4.42 0 as K1
Node displacement Nearest Location 3.09 4.76 0 as K2
Node displacement Nearest Location 3.39 5.06 0 as K3
Node displacement Nearest Location 4.03 5.70 0 as K4
Node displacement Nearest Location 6.19 7.86 0 as K5
Node displacement Nearest Location 9.21 10.88 0 as K6
Node displacement Nearest Location 13.54 15.21 0 as K7
Node displacement Nearest Location 0.00 4.42 0 as L1
Node displacement Nearest Location 0.00 4.88 0 as L2
Node displacement Nearest Location 0.00 5.33 0 as L3
Node displacement Nearest Location 0.00 6.25 0 as L4
Node displacement Nearest Location 0.00 9.30 0 as L5
Node displacement Nearest Location 0.00 13.56 0 as L6
Node displacement Nearest Location 0.00 15.21 0 as L7
Node displacement Nearest Location 2.75 0.30 0 as M1
Node displacement Nearest Location 3.66 0.30 0 as M2
Node displacement Nearest Location   4.58   0.30  0  as M3
Node displacement Nearest Location   7.63   0.30  0  as M4
Node displacement Nearest Location   11.89  0.30  0  as M5
Node displacement Nearest Location   17.99  0.30  0  as M6
Node displacement Nearest Location   2.75  -0.78  0  as N2
Node displacement Nearest Location   2.75   4.12  0  as O1
Node displacement Nearest Location   17.99  -0.78  0  as N1
Node displacement Nearest Location   17.99  4.12  0  as O2

Element stress Nearest Location   0.00   -1.08  -0.14  as P1
Element stress Nearest Location   0.00   -4.73  -0.14  as P2
Element stress Nearest Location   0.46   -1.08  -0.14  as Q1
Element stress Nearest Location   0.46   -8.69  -0.14  as Q2
Element stress Nearest Location   0.46  -16.32  -0.14  as Q3
Element stress Nearest Location   2.75    1.21  -0.14  as R1
Element stress Nearest Location  10.36    1.21  -0.14  as R2
Element stress Nearest Location   17.99    1.21  -0.14  as R3
Element stress Nearest Location   2.75    1.67  -0.14  as S1
Element stress Nearest Location   6.40    1.67  -0.14  as S2
Element stress Nearest Location   9.14    1.67  -0.14  as S3
Element stress Nearest Location  13.11    1.67  -0.14  as S4
Element stress Nearest Location  24.08    1.67  -0.14  as S5
Element stress Nearest Location   2.75    2.13  -0.14  as T1
Element stress Nearest Location  10.36    2.13  -0.14  as T2
Element stress Nearest Location   17.99    2.13  -0.14  as T3
Element stress Nearest Location   0.46    4.42  -0.14  as U1
Element stress Nearest Location   0.46   12.03  -0.14  as U2
Element stress Nearest Location   0.46   19.66  -0.14  as U3
Element stress Nearest Location   0.00    4.42  -0.14  as V1
Element stress Nearest Location   0.00    8.07  -0.14  as V2

End History Output adagio_history

################################################
####### MECHANICAL INITIAL CONDITIONS ##########
################################################

Begin Initial Condition initialize_temperatureTemp
Include All Blocks
Initialize Variable Name = Temperature
Variable Type = Node
Magnitude = 300
End Initial Condition initialize_temperatureTemp

# Hydrostatic pressure initial condition (varies according to y-direction)
Begin initial condition initialize_stress_state
Initialize variable name = unrotated_stress
Variable type = element
Include All Blocks
Element Block Subroutine = geo_is
Subroutine Real Parameter: bot = -54.19
Subroutine Real Parameter: top = 52.87
Subroutine Real Parameter: po = -15980670.02
Subroutine Real Parameter: p1 = -13570000
Subroutine Real Parameter: kvert_xx = 1
Subroutine Real Parameter: kvert_yy = 1
Subroutine Real Parameter: kvert_zz = 1
Subroutine Real Parameter: kvert_xy = 0
Subroutine Real Parameter: kvert_yz = 0
Subroutine Real Parameter: kvert_zx = 0
Subroutine String Parameter: dir = Y
End initial condition initialize_stress_state

Begin gravity Adagio_gravity
Include all blocks
Direction = y
Gravitational constant = 9.79
Scale Factor = -1.0
Function = gravitational_acceleration_function
End gravity Adagio_gravity

########################################################################
####### MECHANICAL BOUNDARY CONDITIONS #########
########################################################################

# 0 <= x <= 50 m; y=52.87 m
# Lithostatic pressure condition along top-side mesh (surface ID=2001)
Begin pressure
    Surface = surface_2001
    Scale Factor = 1.0
    Function = lithostatic_pressure_ytop_function
End pressure

# 0 <= x <= 50 m; y=-54.19 m
# Lithostatic pressure condition along bottom-side mesh (surface ID=2000)
Begin pressure
    Surface = surface_2000
    Scale Factor = 1.0
    Function = lithostatic_pressure_ybot_function
End pressure

# x=50 m; 49.38 m <= y <= +52.87 m; no xy-displacement; Anhydrite 7
# Fixed displacement condition along right-side mesh
Begin fixed displacement
    Components = x y z
    Components = x y
    Node Set = nodelist_101
End fixed displacement

# x=0 symmetry; no x-displacement
# Fixed x-displacement condition along left-side mesh
Begin fixed displacement
    Components = x
    Node Set = nodelist_100
End fixed displacement

# x=50 m; -54.19 m <= y 49.38 m; no x-displacement
# Fixed x-displacement condition along right-side mesh
Begin fixed displacement
    Components = x
    Node Set = nodelist_102
End fixed displacement

# z=0.0 m; 2D plane strain condition; no z-displacement
# Fixed z-displacement condition along z-bottom mesh
Begin fixed displacement
    Components = z
    Node Set = nodelist_400
End fixed displacement

# z=-0.28 m; 2D plane strain condition; no z-displacement
# Fixed z-displacement condition along z-top mesh
Begin fixed displacement
    Components = z
    Node Set = nodelist_401
End fixed displacement

End Adagio Region AdagioRegion
End Procedure arpeggio_procedure

END SIERRA WIPP_Room_B_Thermal_Structural_Funded_By_UFD
APPENDIX H: HEATED ROOM COUPLED CALCULATION #3
(DIRICHLET TEMPERATURE BOUNDARY CONDITION) INPUT DECK

# directory : /scratch/jsrath/NEAMS/roomb/coupled/simu1003
# file    : arpeggio.i
# author  : Jonathan Scott Rath
# description : UFD 2012 WIPP Room B input deck
# UFD = Used Fuels Disposition
# WIPP = Waste Isolation Pilot Plant = WIPP
# SIERRA = Sandia Integrated Environment for Robust Research Algorithms
# SIERRA Thermal-Mechanical (Aria-Adagio) Calculation
# SIERRA TM WIPP Room B Two-Way Coupled Calculation
# Model 3 (Room B, Thermal+Mechanical)
# revision_log : 06/AUGUST/2012
# - Shifted Dirichlet Temperature B.C. for DHLW power
#   on time (325 days of unheated, T=300 Kelvin)
# - 01/AUGUST/2012
#   - Modified for Dirichlet Temperature B.C. on ROOM B
# - 22/MARCH/2012
#   - Added material AIR
#   - Modified for Dirichlet Temperature B.C. on ROOM B
# - 09/MARCH/2012
# - Modified time stepping for Adagio and Aria region
# - 01/MARCH/2012
# - Implemented new Sam Subia advised Enclosure
#   Radiation approach and method utilizing partial enclosure constructs, etc.
# - 29/FEBRUARY/2012
# - Adapted new syntax for THERMAL STRAIN X FUNCTION
# - Adapted new syntax for THERMAL STRAIN Y FUNCTION
# - Adapted new syntax for THERMAL STRAIN Z FUNCTION
# - Using THERMAL LOG STRAIN X FUNCTION
# - Using THERMAL LOG STRAIN Y FUNCTION
# - Using THERMAL LOG STRAIN Z FUNCTION
# - Adapted heat flux at Room B opening to account
#   for normal outward direction
# - Added convection heat transfer boundary condition
#   (Side Set 4000, h=0.51 W/m^2/K)
# - Added 3dHex8_MESH & 3dHex27_MESH variable control
# - Added non-conditional function tpf.include
# - Added non-conditional function ntc.include
# - Added coefficient of thermal expansion
# - Added power law thermal conductivity form
# - First Edition for "TM"
# unit system : System International (SI)
# mass       = kilogram (kg)
# length     = meter (m)
# time       = seconds (sec)
# Temperature = Kelvin
# density    = kg/(m^3)
# velocity   = meter/sec = 10^-3*km/sec
# acceleration = m/(sec^2)
# force      = mass * acceleration = kg*m/sec^2
# pressure   = Newton / (m^2)
# = Pascal
# energy     = Newton*m
# = Joule
# power      = Joule/sec
BEGIN SIERRA WIPP Room B Thermal_Structural Funded_By_UFD

Begin diagnostic control Adagio_Diagnostics
enable "tangent"
End diagnostic control Adagio_Diagnostics

title UFD WIPP Room B Coupled Thermal-Structural Response Simulation

define direction x with vector 1.0 0.0 0.0
define direction y with vector 0.0 1.0 0.0
define direction z with vector 0.0 0.0 1.0

define direction dir_1 with vector 0.7071067812 0.0 0.7071067812
define direction dir_2 with vector -0.7071067812 0.0 -0.7071067812

define point origin with coordinates 0.0 0.0 0.0

################################################
############### USER PLUG INS ####################
################################################
Load User Plugin File t_dirich3.so

################################################
################ GLOBAL CONSTANTS ###############
################################################
Begin Global Constants
Stefan Boltzmann Constant = 5.67e-08 # [watt (Nm/s)]/(meter^2*degK^4)
End

################################################
################# DATA BLOCKS ###################
################################################
Begin Data Block t_dirich_variables

Integer t_dirich_size = 19

Real t_dirich_times = 0.0000E+00 2.8080E+07 3.3080E+07 3.8080E+07 4.8080E+07 
5.8080E+07 6.8080E+07 7.8080E+07 8.8080E+07 9.8080E+07 
1.0808E+08 1.1808E+08 1.2808E+08 1.3808E+08 1.4808E+08 
1.5808E+08 1.6808E+08 1.7808E+08 1.8808E+08

Real t_dirich_floor = 300.00 300.00 307.00 311.50 316.50 
319.20 321.50 324.60 325.20 
325.50 325.60 325.70 325.75 325.80 
325.85 325.90 325.95 326.00

Real t_dirich_roof = 300.00 300.00 309.00 313.50 320.00 
323.90 326.50 328.40 329.60 330.20 
330.50 330.60 330.70 330.75 330.80 
330.85 330.90 330.95 331.00

End Data Block t_dirich_variables

################################################
################ FUNCTION DEFINITIONS ############
################################################
# WIPP room B floor elevation, y=-1.08 m

Begin Definition for Function t_floor
Type is Piecewise Linear
Begin Values
0.0000E+00 300.00
2.8080E+07 300.00
3.3080E+07 307.00
3.8080E+07 311.50
4.8080E+07 316.50
5.8080E+07 319.20
6.8080E+07 321.50
7.8080E+07 323.40
8.8080E+07 324.60
9.8080E+07 325.20
1.0808E+08 325.50
1.1808E+08 325.60
1.2808E+08 325.70
1.3808E+08 325.75
1.4808E+08 325.80
1.5808E+08 325.85
1.6808E+08 325.90
1.7808E+08 325.95
1.8808E+08 326.00
End Values

End Definition for Function t_floor

# WIPP room B roof elevation, y=4.42 m

Begin Definition for Function t_roof
Type is Piecewise Linear
Begin Values
0.0000E+00 300.00
2.8080E+07 300.00
3.3080E+07 309.00
3.8080E+07 313.50
4.8080E+07 320.00
5.8080E+07 323.90
6.8080E+07 326.50
7.8080E+07 328.40
8.8080E+07 329.60
9.8080E+07 330.20
1.0808E+08 330.50
1.1808E+08 330.60
1.2808E+08 330.70
1.3808E+08 330.75
1.4808E+08 330.80
1.5808E+08 330.85
1.6808E+08 330.90
1.7808E+08 330.95
1.8808E+08 331.00
End Values

End Definition for Function t_roof
begin definition for function gravitational_acceleration_function

begin values

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>157784630.4</td>
<td>1</td>
</tr>
</tbody>
</table>

end values

end definition for function gravitational_acceleration_function

begin definition for function lithostatic_pressure_ybot_function

begin values

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>15780670.02</td>
</tr>
<tr>
<td>157784630.4</td>
<td>15780670.02</td>
</tr>
</tbody>
</table>

end values

end definition for function lithostatic_pressure_ybot_function

begin definition for function lithostatic_pressure_ytop_function

begin values

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1357000</td>
</tr>
<tr>
<td>157784630.4</td>
<td>1357000</td>
</tr>
</tbody>
</table>

end values

end definition for function lithostatic_pressure_ytop_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 2.4e-05 [1/Kelvin]
# ----------------------------
# T_ref    0.0
# T_max    (T_max-T_ref)*alpha
# ----------------------------

begin definition for function polyhalite_thermal_strain_function

begin values

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>0</td>
</tr>
<tr>
<td>1500</td>
<td>0.0288</td>
</tr>
</tbody>
</table>

end values

end definition for function polyhalite_thermal_strain_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 4e-05 [1/Kelvin]
# ----------------------------
# T_ref    0.0
# T_max    (T_max-T_ref)*alpha
# ----------------------------

begin definition for function argillaceous_thermal_strain_function

begin values

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>0</td>
</tr>
<tr>
<td>1500</td>
<td>0.048</td>
</tr>
</tbody>
</table>

end values

end definition for function argillaceous_thermal_strain_function

# T_ref = 300 [Kelvin]
# T_max = 1500 [Kelvin]
# alpha = 2e-05 [1/Kelvin]
# ----------------------------
# T_ref    0.0
# T_max    (T_max-T_ref)*alpha
# ----------------------------

begin definition for function anhydrite_thermal_strain_function

begin values
Begin solid section hex8
  Strain Incrementation = midpoint_increment
  Hourglass rotation = scaled
End solid section hex8

Begin Property Specification for material polyhalite
  Density = 2300
  thermal log strain x function = polyhalite_thermal_strain_function
  thermal log strain y function = polyhalite_thermal_strain_function
  thermal log strain z function = polyhalite_thermal_strain_function
End definition for function polyhalite_thermal_strain_function

Begin definition for function halite_thermal_strain_function
  Type is piecewise linear
  Begin values
    300 0
    1500 0.054
  End values
End definition for function halite_thermal_strain_function

Begin definition for function polyhalite_pressure_volstrain_function
  Type is piecewise linear
  Ordinate is volumetric_strain
  Abscissa is Pressure
  Begin values
    -1 -6.583333333e+10 # -65833.33333 MPa
    0 0
    1 6.583333333e+10 # 65833.33333 MPa
  End values
End definition for function polyhalite_pressure_volstrain_function

Begin definition for function anhydrite_pressure_volstrain_function
  Type is piecewise linear
  Ordinate is volumetric_strain
  Abscissa is Pressure
  Begin values
    -1 -8.344444444e+10 # -83444.44444 MPa
    0 0
    1 8.344444444e+10 # 83444.44444 MPa
  End values
End definition for function anhydrite_pressure_volstrain_function
#bulk modulus = 6.583333333e+10 # [Pa]
#shear modulus = 2.033088235e+10 # [Pa]
a0 = 2459512.147 # [Pa]
a1 = 2.457780096
a2 = 0 # [1/Pa]
pressure cutoff = -1000704.722 # [Pa]
pressure function = polyhalite_pressure_volstrain_function
End Parameters for model soil_foam
End Property Specification for material polyhalite

Begin Property Specification for material argillaceous
Density = 2300
thermal log strain x function = argillaceous_thermal_strain_function
thermal log strain y function = argillaceous_thermal_strain_function
thermal log strain z function = argillaceous_thermal_strain_function
Begin Parameters For Model MD_Creep
# Youngs Modulus = 3.100000833e+10
# Poissons Ratio = 0.250000336
# Lambda = 1.240003333e+10
# Two Mu = 2.48e+10
Bulk Modulus = 2.06667e+10
Shear Modulus = 1.24e+10
A1 = 1.406e+23
Q1/R = 12581.78
# Q1/RT = 41.93326667 # Isothermal, T=300 Kelvin
N1 = 5.5
B1 = 8993300
A2 = 1.3131e+13
Q2/R = 5032.71
# Q2/RT = 16.7757 # Isothermal, T=300 Kelvin
N2 = 5
B2 = 0.042875
Sig0 = 20570000
Qlc = 5335
M = 3
K0 = 2470000
# CSTAR = 0.009189
# TK = 300
# C = 2.759 # C = CSTAR/TK (MD Creep model uses C when isothermal)
C = 0.009189 # C = CSTAR/TK (MD Creep model uses C=CSTAR when nonisothermal)
Alpha = -14.96
Beta = -7.738
Deltaclc = 0.58
Amult = 0.5
Grwfac = 1.05
Epstol = 0.005
Shkfac = 1
Itype = 0
Angle = 0.1
End Parameters For Model MD_Creep
End Property Specification for material argillaceous

Begin Property Specification for material anhydrite
Density = 2300
thermal log strain x function = anhydrite_thermal_strain_function
thermal log strain y function = anhydrite_thermal_strain_function
thermal log strain z function = anhydrite_thermal_strain_function
Begin parameters for model soil_foam
youngs modulus = 7.51e+10 # [Pa]
poissons ratio = 0.35 # [dimensionless]
# bulk modulus = 8.344444444e+10 # [Pa]
shear modulus = 2.781481481e+10 # [Pa]
a0 = 2338268.59 # [Pa]
a1 = 2.33826859
a2 = 0 # [1/Pa]
pressure cutoff = -1000000 # [Pa]
pressure function = anhydrite_pressure_volstrain_function
End Parameters for model soil_foam
End Property Specification for material anhydrite

Begin Property Specification for material halite
Density = 2300
thermal log strain x function = halite_thermal_strain_function
thermal log strain y function = halite_thermal_strain_function
thermal log strain z function = halite_thermal_strain_function

Begin Parameters For Model MD_Creep
# Youngs Modulus = 3.1e+10
# Poissons Ratio = 0.25
# Lambda = 1.24e+10
# Two Mu = 2.48e+10
Bulk Modulus = 2.066666667e+10
Shear Modulus = 1.24e+10
A1 = 8.386e+22
Q1/R = 12581.78158
# Q1/RT = 41.93927193 # Isothermal, T=300 Kelvin
N1 = 5.5
B1 = 6086000
A2 = 9.672e+12
Q2/R = 5032.712632
# Q2/RT = 16.77570877 # Isothermal, T=300 Kelvin
N2 = 5
B2 = 0.03034
Sig0 = 20570000
Qlc = 5335
M = 3
K0 = 627500
# CSTAR = 0.009189
# TK = 300
# C = 2.759 # C = CSTAR/TK (MD Creep model uses C when isothermal)
# C = 0.009189 # C (MD Creep model uses C=CSTAR when nonisothermal)
Alpha = -17.37
Beta = -7.738
Deltalc = 0.58
Amult = 0.5
Grwfac = 1.05
Epstol = 0.005
Shkfac = 1
Itype = 0
Angle = 0.1
End Parameters For Model MD_Creep
End Property Specification for material halite

Begin Aria Material ONE
Density = Constant Rho = 2300 # [kg/m^3]
Thermal Conductivity = Power_law A = 3333.406168 gamma = -1.14
Specific heat = Constant Cp = 860 # [joule (Nm)]/(kilogram*degK)
Emissivity = Constant e = 0.8 # [1]
Heat Conduction = basic
End Aria Material ONE

########################################################################
Begin Finite Element Model Adagio_FEM

Database Name = roomb.g
Database Type = exodusII

Begin parameters for block block_1
   material polyhalite
   solid mechanics use model soil_foam
   section = hex8
   hourglass stiffness = 0.003
End Parameters for block block_1

Begin parameters for block block_2
   material argillaceous
   solid mechanics use model MD_Creep
   section = hex8
   hourglass stiffness = 0.003
End Parameters for block block_2

Begin parameters for block block_3
   material anhydrite
   solid mechanics use model soil_foam
   section = hex8
   hourglass stiffness = 0.003
End Parameters for block block_3

Begin parameters for block block_4
   material halite
   solid mechanics use model MD_Creep
   section = hex8
   hourglass stiffness = 0.003
End Parameters for block block_4

End Finite Element Model Adagio_FEM

Begin Finite Element Model Aria_FEM

Database Name = roombq.g
Database Type = exodusII
Coordinate System is cartesian

Use Material ONE for block_1
#
# Material TWO not used in coupled thermal-structural calculation (arpeggio).
# (previously known as "thermal equivalent material")
#
# Omit Volume block_2
# Use Material TWO for block_2
#

End Finite Element Model Aria_FEM

Begin Aztec Equation Solver AriaLinearEquationSolverAztec
   Solution Method = cg
   Preconditioning Method = DD-ICC
   Maximum Iterations = 500

End Aztec Equation Solver AriaLinearEquationSolverAztec
Residual Norm Tolerance = 1e-08
Residual Norm Scaling = r0
End Aztec Equation Solver AriaLinearEquationSolverAztec

Begin Trilinos Equation Solver AriaLinearEquationSolverTrilinos
Solution Method = cg
Preconditioning Method = multilevel #jacobi
Maximum Iterations = 2000
Residual Norm Scaling = r0
Residual Norm Tolerance = 1.0e-08
End Trilinos Equation Solver AriaLinearEquationSolverTrilinos

########################################################################
# ARPEGGIO PROCEDURE #
########################################################################

Begin Procedure arpeggio_procedure

Begin Solution Control Description
Use System Main

Begin System Main
Simulation Start Time            = 0
Simulation Termination Time      = 157784630.4 # 5 [years] = 1826.211 [days]
Simulation Max Global Iterations = 1e+12
Begin Transient Time_Block_1
Advance AriaRegion
  Transfer Aria_to_Adagio
  Advance AdagioRegion
  Transfer Adagio_to_Aria
End Transient Time_Block_1
Begin Transient Time_Block_2
Advance AriaRegion
  Transfer Aria_to_Adagio
  Advance AdagioRegion
  Transfer Adagio_to_Aria
End Transient Time_Block_2
End System Main

Begin Parameters For Transient Time_Block_1
Start Time = 0
Termination Time = 28080000 # 0.8898205081 [years] = 325 [days]
Begin Parameters For Aria Region AriaRegion
  Time Integration Method = Second_Order
  Time Step Variation = Adaptive
  Initial Time Step Size = 1e-06
  Minimum Time step Size = 5e-07
  Maximum Time step Size = 26055 # 0.00082565076 [years] = 0.3015625 [days]
  Maximum Time Step Size ratio = 10
  Minimum Resolved Time Step Size = 5e-07
  Predictor-Corrector Tolerance = 0.0005
  Predictor-Corrector Normalization = MAX
End Parameters for Aria Region AriaRegion
Begin parameters for Adagio Region AdagioRegion
  Time Increment = 1e-06
End Parameters for Adagio Region AdagioRegion
End Parameters for Transient Time_Block_1

Begin Parameters For Transient Time_Block_2
Start Time = 28080000 # 0.8898205081 [years] = 325 [days]
Termination Time = 157784630.4 # 5 [years] = 1826.211 [days]

Begin Parameters For Aria Region AriaRegion
  Time Integration Method = Second_Order
  Time Step Variation = Adaptive
  Initial Time Step Size = 100 # 3.1687645e-06 [years] =
  0.001157407407 [days]
  Minimum Time step Size = 50
  Maximum Time step Size = 864000 # 0.02737909256 [years] = 10 [days]
  Maximum Time Step Size ratio = 10
  Minimum Resolved Time Step Size = 50
  Predictor-Corrector Tolerance = 0.0005
  Predictor-Corrector Normalization = MAX
End Parameters For Aria Region AriaRegion

Begin parameters for Adagio Region AdagioRegion
  Time Increment = 100 # 3.168876454e-06 [years] =
  0.001157407407 [days]
End Parameters for Adagio Region AdagioRegion
End Parameters For Transient Time_Block_2

End Solution Control Description

#########################################################################
######## SIERRA CODE TO CODE TRANSFERS ##############
#########################################################################

Begin Transfer Aria_to_Adagio
  Interpolate Volume Nodes from AriaRegion to AdagioRegion
  Send Field Solution->Temperature State New to Temperature State New
  Search Coordinate Field model_coordinates state none to model_coordinates state none
  Send Block block_1 to block_1 block_2 block_3 block_4
End Transfer Aria_to_Adagio

Begin Transfer Adagio_to_Aria
  Interpolate Volume Nodes from AdagioRegion to AriaRegion
  Send Field Displacement State New to Solution->Mesh_Displacements State New
  Search Coordinate Field model_coordinates state none to model_coordinates
  state none
  Send Block block_1 block_2 block_3 block_4 to block_1
End Transfer Adagio_to_Aria

#########################################################################
################## ARIA REGION ##########################################
#########################################################################

Begin Aria Region AriaRegion
  Use Data Block t_dirich_variables
  Use Finite Element Model Aria_FEM
  Use Linear Solver AriaLinearEquationSolverAztec
  Nonlinear Solution Strategy = Newton
  NONLINEAR RESIDUAL TOLERANCE = 1.0e-6
  MAXIMUM NONLINEAR ITERATIONS = 5
  NONLINEAR RELAXATION FACTOR = 1.0
  Use DOF Averaged Nonlinear Residual
  Accept Solution After Maximum Nonlinear Iterations = true

#########################################################################
 autonomy GOVERNING EQUATIONS autonomy
#########################################################################
EQ Energy for Temperature on All_blocks using Q1 with Lumped_Mass DIFF
SRC
EQ Mesh for Mesh_Displacements on All_blocks using Q1 with Xfer
#
(Only block_1 in FY2012 coupled thermal-structural simulations)
SRC
EQ Energy for Temperature on block_1 using Q1 with Lumped_Mass DIFF
SRC
EQ Mesh for Mesh_Displacements on block_1 using Q1 with Xfer
#
(No block_2, previously known as the "equivalent thermal material")
SRC
EQ Energy for Temperature on block_2 using Q1 with Lumped_Mass DIFF
SRC
EQ Mesh for Mesh_Displacements on block_2 using Q1 with Xfer

PostProcess HEAT_FLUX on All_Blocks using Q1

################################################
########## THERMAL INITIAL CONDITIONS ##########
################################################
IC CONST on All_blocks Temperature = 300

################################################
########## THERMAL BOUNDARY CONDITIONS ##########
################################################
# Adiabatic or Isentropic BC (i.e., "von Neuman") energy flux = 0
# von Neuman B.C. left symmetry
BC Flux for Energy on surface_1000 = constant flux = 0.0
# von Neuman B.C. right far-field
BC Flux for Energy on surface_1001 = constant flux = 0.0
# von Neuman B.C. y-vertical bottom model
BC Flux for Energy on surface_2000 = constant flux = 0.0
# von Neuman B.C. y-vertical top model
BC Flux for Energy on surface_2001 = constant flux = 0.0
# Dirichlet B.C. on WIPP Room B Floor, y=-1.08 m
BC Dirichlet for Temperature on surface_4001 = User_Function name=t_floor
X=Time
# Dirichlet B.C. on WIPP Room B Pillar, -1.08 m <= y <= 4.42 m
BC Dirichlet for Temperature on surface_4002 = Calore_User_Sub Name=dirich_bc
type=node
# Dirichlet B.C. on WIPP Room B Roof, y=4.42 m
BC Dirichlet for Temperature on surface_4003 = User_Function Name=t_roof
X=Time

################################################
############## SURFACE HEAT SOURCE ##############
################################################
# BC Flux for Energy on surface_6666 = Function Name = DHLW_power_flux_function
Begin Heat Flux Boundary Condition Aria_DHLW
  Add Surface surface_6666
  Flux Time Function = DHLW_power_flux_function
End Heat Flux Boundary Condition Aria_DHLW

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### ARIA SIMULATION OUTPUT RESULTS

**Begin Results Output output_Aria**

Database Name = roombq.e
Database Type = ExodusII

Global Variables = time_step as timestep
Global Variables = encl_roombq_power
Global Variables = encl_roombq_flux

Nodal Variables = solution->mesh_displacements as displ
Nodal Variables = solution->temperature as temp
Nodal Variables = pp->HEAT_FLUX as heatflux

Timestep Adjustment Interval = 4

At time 0, Increment = 604800 # ( t=0 seconds, incr=1 weeks )
At time 15778463.04, Increment = 2629743.84 # ( t=0.5 years, incr=1 months )
At time 31556926.08, Increment = 2629743.84 # ( t=1 years, incr=1 months )
At time 63113852.16, Increment = 2629743.84 # ( t=2 years, incr=1 months )
At time 94670778.24, Increment = 2629743.84 # ( t=3 years, incr=1 months )
At time 126227704.3, Increment = 2629743.84 # ( t=4 years, incr=1 months )
At time 157784630.4, Increment = 2629743.84 # ( t=5 years, incr=1 months )

Termination Time = 157784630.4 # 5 years

**End Results Output output_Aria**

### ARIA SIMULATION HISTORY RESULTS

**Begin History Output history_output_Aria**

Database Name = roombq.h
Database Type = ExodusII

At time 0, Increment = 604800 # ( t=0 seconds, incr=1 weeks )
At time 15778463.04, Increment = 2629743.84 # ( t=0.5 years, incr=1 months )

At time 31556926.08, Increment = 2629743.84 # ( t=1 years, incr=1 months )
At time 63113852.16, Increment = 2629743.84 # ( t=2 years, incr=1 months )
At time 94670778.24, Increment = 2629743.84 # ( t=3 years, incr=1 months )
At time 126227704.3, Increment = 2629743.84 # ( t=4 years, incr=1 months )
At time 157784630.4, Increment = 2629743.84 # ( t=5 years, incr=1 months )

Termination Time = 157784630.4 # 5 years

**End History Output history_output_Aria**
Node solution->temperature Nearest Location 0.21 -4.20 -0.762 as C4
Node solution->temperature Nearest Location 0.21 -5.12 -0.762 as C5
Node solution->temperature Nearest Location 0.21 -6.03 -0.762 as C6
Node solution->temperature Nearest Location 0.21 -6.95 -0.762 as C7
Node solution->temperature Nearest Location 0.40 -1.08 -0.762 as D1
Node solution->temperature Nearest Location 0.40 -2.38 -0.762 as D2
Node solution->temperature Nearest Location 0.40 -3.29 -0.762 as D3
Node solution->temperature Nearest Location 0.40 -4.20 -0.762 as D4
Node solution->temperature Nearest Location 0.40 -5.12 -0.762 as D5
Node solution->temperature Nearest Location 0.40 -6.03 -0.762 as D6
Node solution->temperature Nearest Location 0.40 -6.95 -0.762 as D7
Node solution->temperature Nearest Location 0.76 -1.08 -0.762 as E1
Node solution->temperature Nearest Location 0.76 -2.38 -0.762 as E2
Node solution->temperature Nearest Location 0.76 -3.29 -0.762 as E3
Node solution->temperature Nearest Location 0.76 -4.20 -0.762 as E4
Node solution->temperature Nearest Location 0.76 -5.12 -0.762 as E5
Node solution->temperature Nearest Location 0.76 -6.03 -0.762 as E6
Node solution->temperature Nearest Location 0.76 -6.95 -0.762 as E7
Node solution->temperature Nearest Location 1.13 -1.08 -0.762 as F1
Node solution->temperature Nearest Location 1.31 -1.51 -0.762 as F2
Node solution->temperature Nearest Location 1.49 -1.93 -0.762 as F3
Node solution->temperature Nearest Location 1.83 -2.76 -0.762 as F4
Node solution->temperature Nearest Location 3.01 -5.59 -0.762 as F5
Node solution->temperature Nearest Location 4.63 -9.52 -0.762 as F6
Node solution->temperature Nearest Location 6.98 -15.16 -0.762 as F7
Node solution->temperature Nearest Location 2.75 -1.08 -0.762 as G1
Node solution->temperature Nearest Location 2.75 -1.42 -0.762 as G2
Node solution->temperature Nearest Location 2.75 -1.72 -0.762 as G3
Node solution->temperature Nearest Location 4.03 -2.36 -0.762 as G4
Node solution->temperature Nearest Location 6.19 -4.52 -0.762 as G5
Node solution->temperature Nearest Location 9.21 -7.54 -0.762 as G6
Node solution->temperature Nearest Location 13.54 -11.87 -0.762 as G7
Node solution->temperature Nearest Location 2.75 -0.62 -0.762 as H1
Node solution->temperature Nearest Location 3.21 -0.62 -0.762 as H2
Node solution->temperature Nearest Location 3.66 -0.62 -0.762 as H3
Node solution->temperature Nearest Location 4.58 -0.62 -0.762 as H4
Node solution->temperature Nearest Location 7.63 -0.62 -0.762 as H5
Node solution->temperature Nearest Location 11.89 -0.62 -0.762 as H6
Node solution->temperature Nearest Location 17.99 -0.62 -0.762 as H7
Node solution->temperature Nearest Location 2.75 1.67 -0.762 as I1
Node solution->temperature Nearest Location 3.21 1.67 -0.762 as I2
Node solution->temperature Nearest Location 3.66 1.67 -0.762 as I3
Node solution->temperature Nearest Location 4.58 1.67 -0.762 as I4
Node solution->temperature Nearest Location 7.63 1.67 -0.762 as I5
Node solution->temperature Nearest Location 11.89 1.67 -0.762 as I6
Node solution->temperature Nearest Location 17.99 1.67 -0.762 as I7
Node solution->temperature Nearest Location 2.75 3.96 -0.762 as J1
Node solution->temperature Nearest Location 3.21 3.96 -0.762 as J2
Node solution->temperature Nearest Location 3.66 3.96 -0.762 as J3
Node solution->temperature Nearest Location 4.58 3.96 -0.762 as J4
Node solution->temperature Nearest Location 7.63 3.96 -0.762 as J5
Node solution->temperature Nearest Location 11.89 3.96 -0.762 as J6
Node solution->temperature Nearest Location 17.99 3.96 -0.762 as J7
Node solution->temperature Nearest Location 2.75 4.42 -0.762 as K1
Node solution->temperature Nearest Location 3.09 4.76 -0.762 as K2
Node solution->temperature Nearest Location 3.39 5.06 -0.762 as K3
Node solution->temperature Nearest Location 4.03 5.70 -0.762 as K4
Node solution->temperature Nearest Location 6.19 7.86 -0.762 as K5
Node solution->temperature Nearest Location 9.21 10.88 -0.762 as K6
Node solution->temperature Nearest Location 13.54 15.21 -0.762 as K7
Node solution->temperature Nearest Location 0.00 4.42 -0.762 as L1
Node solution->temperature Nearest Location 0.00 4.88 -0.762 as L2
Node solution->temperature Nearest Location 0.00 5.33 -0.762 as L3
| Node solution->temperature Nearest Location   | 0.00 | 6.25 | -0.762 | as L4 |
| Node solution->temperature Nearest Location   | 0.00 | 9.30 | -0.762 | as L5 |
| Node solution->temperature Nearest Location   | 0.00 | 13.56 | -0.762 | as L6 |
| Node solution->temperature Nearest Location   | 0.00 | 15.21 | -0.762 | as L7 |
| Node solution->temperature Nearest Location   | 0.00 | 5.02 | -0.762 | as AB6 |
| Node solution->temperature Nearest Location   | 0.00 | 5.32 | -0.762 | as AB5 |
| Node solution->temperature Nearest Location   | 0.00 | 6.22 | -0.762 | as AB4 |
| Node solution->temperature Nearest Location   | 0.00 | 9.32 | -0.762 | as AB3 |
| Node solution->temperature Nearest Location   | 0.00 | 13.62 | -0.762 | as AB2 |
| Node solution->temperature Nearest Location   | 0.00 | 19.72 | -0.762 | as AB1 |
| Node solution->temperature Nearest Location   | 0.00 | -1.68 | -0.762 | as BE6 |
| Node solution->temperature Nearest Location   | 0.00 | -1.98 | -0.762 | as BE5 |
| Node solution->temperature Nearest Location   | 0.00 | -2.88 | -0.762 | as BE4 |
| Node solution->temperature Nearest Location   | 0.00 | -5.98 | -0.762 | as BE3 |
| Node solution->temperature Nearest Location   | 0.00 | -10.28 | -0.762 | as BE2 |
| Node solution->temperature Nearest Location   | 0.00 | -16.38 | -0.762 | as BE1 |

End History Output history_output_Aria

End Aria Region AriaRegion

################################
# ADAGIO REGION #
################################

Begin Adagio Region AdagioRegion

Use Finite Element Model adagio_FEM

Begin adaptive time stepping Adagio_ATS
  target iterations = 500
  method = material # <solver> | material
  cutback factor = 0.5 # <0.5>
  growth factor = 1.05 # <1.5>
  minimum multiplier = 0.0001
  maximum multiplier = 1e+14
  maximum failure cutbacks = 10 # <5>
  iteration window = 5 # <target_iterations/10>
End adaptive time stepping Adagio_ATS

Begin solver Adagio_solver

  Level 1 Predictor = default # none | <default>

Begin Control Contact Adagio_Control_Contact
  Level = 1
  Target Relative Residual = 0.005
  Acceptable Relative Residual = 100
  Minimum Iterations = 1
  Maximum Iterations = 1000
  Reference = EXTERNAL # <EXTERNAL> | INTERNAL

| BELYTSCHKO | RESIDUAL | ENERGY |

End Control Contact Adagio_Control_Contact

Begin loadstep predictor Adagio_Loadstep_Predictor
  type = scale_factor
  scale factor = 1.0 0.0
End loadstep predictor Adagio_Loadstep_Predictor

Begin cg Adagio_CG
  Line Search Tangent
    Target Relative Residual = 0.0005
    Acceptable Relative Residual = 0.01

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# Iteration Reset = 10 # <10000>
Iteration Print = 400
Minimum Iterations = 1
Maximum Iterations = 50000
Preconditioner = diagonal # <elastic> | block_initial
| probe | schur | diagonal
Balance Probe = 1 # <0> | 1 | 2
Nodal Probe Factor = 1e-06 # <1.0e-06>
Beta Method = PolakRibierePlus # <PolakRibiere> |
PolakRibierePlus | FletcherReeves
End cg Adagio_CG
End solver Adagio_solver

################################################
## ADAGIO CONTACT DEFINITIONS
################################################

Begin Contact Definition Adagio_WIPP_Room_B_Clay_Seams

Enforcement = Frictional

Contact Surface surf_3000 contains surface_3000
Contact Surface surf_3001 contains surface_3001
Contact Surface surf_3002 contains surface_3002
Contact Surface surf_3003 contains surface_3003
Contact Surface surf_3004 contains surface_3004
Contact Surface surf_3005 contains surface_3005
Contact Surface surf_3006 contains surface_3006
Contact Surface surf_3007 contains surface_3007
Contact Surface surf_3008 contains surface_3008
Contact Surface surf_3009 contains surface_3009
Contact Surface surf_3010 contains surface_3010
Contact Surface surf_3011 contains surface_3011
Contact Surface surf_3012 contains surface_3012
Contact Surface surf_3013 contains surface_3013
Contact Surface surf_3014 contains surface_3014
Contact Surface surf_3015 contains surface_3015
Contact Surface surf_3016 contains surface_3016
Contact Surface surf_3017 contains surface_3017

Begin Interaction Clay_D
Master = surf_3000
Slave = surf_3001
  Normal Tolerance = 0.01
  Tangential Tolerance = 0.1
  Capture Tolerance = 0.01
  Tension Release = 1e+20
  Friction Coefficient = 0.2
End Interaction Clay_D

Begin Interaction Clay_E
Master = surf_3002
Slave = surf_3003
  Normal Tolerance = 0.01
  Tangential Tolerance = 0.1
  Capture Tolerance = 0.01
  Tension Release = 1e+20
  Friction Coefficient = 0.2
End Interaction Clay_E

Begin Interaction Clay_F
Master = surf_3004
Slave = surf_3005  
Normal Tolerance = 0.01  
Tangential Tolerance = 0.1  
Capture Tolerance = 0.01  
Tension Release = 1e+20  
Friction Coefficient = 0.2  
End Interaction Clay_F

Begin Interaction Clay_G  
Master = surf_3006  
Slave = surf_3007  
Normal Tolerance = 0.01  
Tangential Tolerance = 0.1  
Capture Tolerance = 0.01  
Tension Release = 1e+20  
Friction Coefficient = 0.2  
End Interaction Clay_G

Begin Interaction Clay_H  
Master = surf_3008  
Slave = surf_3009  
Normal Tolerance = 0.01  
Tangential Tolerance = 0.1  
Capture Tolerance = 0.01  
Tension Release = 1e+20  
Friction Coefficient = 0.2  
End Interaction Clay_H

Begin Interaction Clay_I  
Master = surf_3010  
Slave = surf_3011  
Normal Tolerance = 0.01  
Tangential Tolerance = 0.1  
Capture Tolerance = 0.01  
Tension Release = 1e+20  
Friction Coefficient = 0.2  
End Interaction Clay_I

Begin Interaction Clay_J  
Master = surf_3012  
Slave = surf_3013  
Normal Tolerance = 0.01  
Tangential Tolerance = 0.1  
Capture Tolerance = 0.01  
Tension Release = 1e+20  
Friction Coefficient = 0.2  
End Interaction Clay_J

Begin Interaction Clay_K  
Master = surf_3014  
Slave = surf_3015  
Normal Tolerance = 0.01  
Tangential Tolerance = 0.1  
Capture Tolerance = 0.01  
Tension Release = 1e+20  
Friction Coefficient = 0.2  
End Interaction Clay_K

Begin Interaction Clay_L  
Master = surf_3016  
Slave = surf_3017  
Normal Tolerance = 0.01  
Tangential Tolerance = 0.1
Capture Tolerance = 0.01
Tension Release = 1e+20
Friction Coefficient = 0.2
End Interaction Clay_L

End Contact Definition Adagio_WIPP_Room_B_Clay_Seams

#################################################
####### ADAGIO SIMULATION OUTPUT RESULTS #######
#################################################
Begin Results Output adagio_output
Database Name = roomb.e
Database Type = exodusII
At Time 0 Increment = 600 # Every 10.0 minutes
At Time 3600 Increment = 3600 # Every hour
At Time 86400 Increment = 86400 # Every day
At Time 604800 Increment = 604800 # Every Week
At Time 2629743.84 Increment = 2629743.84 # Every Month
At Time 15778463.04 Increment = 7889231.52 # Every 0.25*year
At Time 15778463.04 Increment = 7889231.52 # Every 0.25*year
Global Variables = timestep as timestep
Global Variables = kinetic_energy as ke
Global Variables = contact_energy as ce
Nodal Variables = velocity as vel
Nodal Variables = displacement as displ
Element Variables = stress as sig
Element Variables = unrotated_stress as usig
Element Variables = von_mises as vonmises
Element Variables = hydrostatic_stress as pressure
Element Variables = stress_invariant_1 as sinv1
Element Variables = stress_invariant_2 as sinv2
Element Variables = stress_invariant_3 as sinv3
Element Variables = max_principal_stress as psgm1
Element Variables = intermediate_principal_stress as psgm2
Element Variables = min_principal_stress as psgm3
Element Variables = max_shear_stress
Element Variables = octahedral_shear_stress as octahedral
Element Variables = temperature as temp
Element Variables = log_strain as strain
Element Variables = log_strain_invariant_1 as volstrain
End Results Output adagio_output

#################################################
###### ADAGIO SIMULATION HISTORY RESULTS #######
#################################################
Begin History Output adagio_history
Database Name = roomb.h
Database Type = exodusII
At Time 0 Increment = 600 # Every 10.0 minutes
At Time 3600 Increment = 3600 # Every hour
At Time 86400 Increment = 86400 # Every day
At Time 604800 Increment = 604800 # Every Week
At Time 2629743.84 Increment = 2629743.84 # Every Month
At Time 15778463.04 Increment = 1314871.92 # Every 0.5*months
At Time 47335389.12 Increment = 7889231.52 # Every 0.25*year

Node displacement Nearest Location   0.0   -1.08  0  as A1
Node displacement Nearest Location   0.0   -1.54  0  as A2
Node displacement Nearest Location   0.0   -1.99  0  as A3
Node displacement Nearest Location   0.0   -2.38  0  as A4
Node displacement Nearest Location   0.0   -3.29  0  as A6
Node displacement Nearest Location   0.0   -4.20  0  as A7
Node displacement Nearest Location   0.0   -5.12  0  as A8
Node displacement Nearest Location   0.0   -5.96  0  as A9
Node displacement Nearest Location   0.0   -6.03  0  as A10
Node displacement Nearest Location   0.0   -6.95  0  as A11
Node displacement Nearest Location   0.0  -10.22  0  as A12
Node displacement Nearest Location   0.0  -16.32  0  as A13
Node displacement Nearest Location  2.75   1.67  0  as I1
Node displacement Nearest Location  3.21   1.67  0  as I2
Node displacement Nearest Location  3.66   1.67  0  as I3
Node displacement Nearest Location  4.58   1.67  0  as I4
Node displacement Nearest Location  7.63   1.67  0  as I5
Node displacement Nearest Location 11.89   1.67  0  as I6
Node displacement Nearest Location 17.99   1.67  0  as I7
Node displacement Nearest Location  2.75   4.42  0  as K1
Node displacement Nearest Location  3.09   4.76  0  as K2
Node displacement Nearest Location  3.39   5.06  0  as K3
Node displacement Nearest Location  4.03   5.70  0  as K4
Node displacement Nearest Location  6.19   7.86  0  as K5
Node displacement Nearest Location  9.21  10.88  0  as K6
Node displacement Nearest Location 13.54  15.21  0  as K7
Node displacement Nearest Location  0.00   4.42  0  as L1
Node displacement Nearest Location  0.00   4.88  0  as L2
Node displacement Nearest Location  0.00   5.33  0  as L3
Node displacement Nearest Location  0.00   6.25  0  as L4
Node displacement Nearest Location  0.00   9.30  0  as L5
Node displacement Nearest Location  0.00  13.56  0  as L6
Node displacement Nearest Location  0.00  15.21  0  as L7
Node displacement Nearest Location  2.75   0.30  0  as M1
Node displacement Nearest Location  3.66   0.30  0  as M2
Node displacement Nearest Location  4.58   0.30  0  as M3
Node displacement Nearest Location  7.63   0.30  0  as M4
Node displacement Nearest Location 11.89   0.30  0  as M5
Node displacement Nearest Location 17.99   0.30  0  as M6
Node displacement Nearest Location  2.75  -0.78  0  as N1
Node displacement Nearest Location  2.75   4.12  0  as O1
Node displacement Nearest Location  2.75  10.36  0  as O2
Element stress Nearest Location   0.00  -1.08  -0.14 as P1
Element stress Nearest Location   0.00  -4.73  -0.14 as P2
Element stress Nearest Location   0.46  -1.08  -0.14 as Q1
Element stress Nearest Location   0.46  -8.69  -0.14 as Q2
Element stress Nearest Location   0.46  -16.32 -0.14 as Q3
Element stress Nearest Location   2.75   1.21  -0.14 as R1
Element stress Nearest Location  10.36  1.21  -0.14 as R2
Element stress Nearest Location 17.99  1.21  -0.14 as R3
Element stress Nearest Location  2.75  1.67  -0.14 as S1
Element stress Nearest Location  6.40  1.67  -0.14 as S2
Element stress Nearest Location  9.14  1.67  -0.14 as S3
Element stress Nearest Location 13.11  1.67  -0.14 as S4
Element stress Nearest Location 24.08  1.67  -0.14 as S5
Element stress Nearest Location  2.75  2.13  -0.14 as T1
Element stress Nearest Location 10.36  2.13  -0.14 as T2
Element stress Nearest Location 17.99  2.13  -0.14 as T3
Element stress Nearest Location  0.46  4.42  -0.14 as U1
Element stress Nearest Location  0.46 12.03  -0.14 as U2
Element stress Nearest Location  0.46 19.66  -0.14 as U3
Element stress Nearest Location  0.00  4.42  -0.14 as V1
Element stress Nearest Location  0.00  8.07  -0.14 as V2

End History Output adagio_history

################################################
####### MECHANICAL INITIAL CONDITIONS ############
################################################

Begin Initial Condition initialize_temperatureTemp
  Include All Blocks
  Initialize Variable Name = Temperature
  Variable Type = Node
  Magnitude = 300
End Initial Condition initialize_temperatureTemp

# Hydrostatic pressure initial condition (varies according to y-direction)
Begin initial condition initialize_stress_state
  Initialize variable name = unrotated_stress
  Variable type = element
  Include All Blocks
  Element Block Subroutine = geo_is
  Subroutine Real Parameter: bot = -54.19
  Subroutine Real Parameter: top = 52.87
  Subroutine Real Parameter: po = -15980670.02
  Subroutine Real Parameter: p1 = -13570000
  Subroutine Real Parameter: kvert_xx = 1
  Subroutine Real Parameter: kvert_yy = 1
  Subroutine Real Parameter: kvert_zz = 1
  Subroutine Real Parameter: kvert_xy = 0
  Subroutine Real Parameter: kvert_yz = 0
  Subroutine Real Parameter: kvert_zx = 0
  Subroutine String Parameter: dir = Y
End initial condition initialize_stress_state

Begin gravity Adagio_gravity
  Include all blocks
  Direction = y
  Gravitational constant = 9.79
  Scale Factor = -1.0
  Function = gravitational_acceleration_function
End gravity Adagio_gravity

################################################
####### MECHANICAL BOUNDARY CONDITIONS ##########
################################################

# 0 <= x <= 50 m; y=52.87 m
# Lithostatic pressure condition along top-side mesh (surface ID=2001)
Begin pressure
  Surface = surface_2001
  Scale Factor = 1.0

Function = lithostatic_pressure_ytop_function
End pressure
#
# 0 <= x <= 50 m; y=-54.19 m
# Lithostatic pressure condition along bottom-side mesh (surface ID=2000)
Begin pressure
  Surface = surface_2000
  Scale Factor = 1.0
  Function = lithostatic_pressure_ybot_function
End pressure
#
# x=50 m; 49.38 m <= y <= +52.87 m; no xy-displacement; Anhydrite 7
# Fixed displacement condition along right-side mesh
Begin fixed displacement
  Components = x y z
  Components = x y
  Node Set = nodelist_101
End fixed displacement
#
# x=0 symmetry; no x-displacement
# Fixed x-displacement condition along left-side mesh
Begin fixed displacement
  Components = x
  Node Set = nodelist_100
End fixed displacement
#
# x=50 m; -54.19 m <= y 49.38 m; no x-displacement
# Fixed x-displacement condition along right-side mesh
Begin fixed displacement
  Components = x
  Node Set = nodelist_102
End fixed displacement
#
# z=0.0 m; 2D plane strain condition; no z-displacement
# Fixed z-displacement condition along z-bottom mesh
Begin fixed displacement
  Components = z
  Node Set = nodelist_400
End fixed displacement
#
# z=-0.28 m; 2D plane strain condition; no z-displacement
# Fixed z-displacement condition along z-top mesh
Begin fixed displacement
  Components = z
  Node Set = nodelist_401
End fixed displacement

End Adagio Region AdagioRegion
End Procedure arpeggio_procedure

END SIERRA WIPP_Room_B_Thermal_Structural_Funded_By_UFD
User Subroutine t_dirich3.C:

```cpp
#include <utility>
#include "math.h"
#include "Aria_Calore_User_Sub_Support.h"

//---------------------------------------------------------
//
//       author : Jonathan Scott Rath
//    directory : /home/jsrath/projects/NEAMS/roomb
//     filename : t_dirich3.C
//      updated : 01/AUGUST/2012
//  description : Used Fuel Disposition (UFD)
//                project FY2012.
//                Waste Isolation Pilot Plant (WIPP)
//                Room B Air Ventilation temperature
//                data interpolation model.
//    references : D.E. Munson, R.L. Jones, J.R. Ball,
//                "Overtest for Simulated Defense
//                High-Level Waste (Room B): In Situ
//                Data Report (May 1984 - February 1989)
//                Waste Isolation Pilot Plant (WIPP)
//                Thermal-Structural Interactions
//                Program", SAND89-2671, Sandia National
//                Laboratories, Albuquerque, NM.
//
//---------------------------------------------------------

int t_pillar_bc(
    UserQuery & user_query,
    Int node_id,             ///< (input)  Node Id
    Int num_nodes,           ///< (input)  number of nodes in nodeset
    Int spatial_dimension,   ///< (input)  spatial dimension
    CoordinateNodes coords,  ///< (input)  coordinates of the nodeset
    DataNodes bc)            ///< (output) array containing the BC values at nodes
{
    // WIPP room B floor elevation, y=-1.08 m
    // WIPP room B roof  elevation, y=4.42 m
    // Roof Temperature function in Array Troof
    // Floor Temperature function in Array Tfloor
    // Time values in Array t

    IntArray1d nsize;
    sierra::String label("t_dirich_size");
    user_query.getUserIntRegionData(nsize, label);

    RealArray1d t;
    sierra::String label1("t_dirich_times");
    user_query.getUserRealRegionData(t, label1);

    RealArray1d Tfloor;
    sierra::String label2("t_dirich_floor");
    user_query.getUserRealRegionData(Tfloor, label2);

    RealArray1d Troof;
    sierra::String label3("t_dirich_roof");
    user_query.getUserRealRegionData(Troof, label3);

    Real time = user_query.currentTime();
```
Real yFloor = -1.08;
Real yRoof = 4.42;

for ( int i = 0; i < nsize(0); i++ ) {
    if ( time >= t(i) &&
         time < t(i+1) )
    {
        Int ilow = i;
        Int ihig = i+1;
        // Interpolate floor temperature at t="time"
        // (Tfloor(ihig)-value)/(Tfloor(ihig)-Tfloor(ilow)) = (t(ihig)-time)/(t(ihig)-
        // t(ilow))
        Real TF = Tfloor(ihig)-((Tfloor(ihig)-Tfloor(ilow))*(t(ihig)-time)/(t(ihig)-
        t(ilow)));
        // Interpolate roof temperature at t="time"
        // (Troof(ihig)-value)/(Troof(ihig)-Troof(ilow)) = (t(ihig)-time)/(t(ihig)-t(ilow))
        Real TR = Troof(ihig)-((Troof(ihig)-Troof(ilow))*(t(ihig)-time)/(t(ihig)-
        t(ilow)));
        for ( int j = 0; j < num_nodes; ++j )
        {
            Real yBC = coords(2, j);
            // Interpolate Temperature at vertical (y-direction) position, yBC:
            // (TR - bc)/(TR - TF) = (yRoof - yBC)/(yRoof - yFloor)
            bc(j) = TR - (TR - TF)*(yRoof - yBC)/(yRoof - yFloor);
        }
    }
    return 0;
}

RegisterFunction(NodeUserSubC, t_pillar_bc, "dirich_bc");
DISTRIBUTION

Federal Agencies

1 US Department of Energy
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   North Las Vegas, NV 89030

1 Waste Isolation Pilot Plant
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   Carlsbad, NM 88220

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   Argonne, IL 60439

1 Los Alamos National Laboratory
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   GERMANY
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