SANDIA REPORT
SAND2012-7525
Unlimited Release
Printed September 2012

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

Jonathan Scott Rath and J. Guadalupe Argüello

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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.

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: http://www.osti.gov/bridge

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd.
Springfield, VA 22161

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.fedworld.gov
Online order: http://www.ntis.gov/help/ordermethods.asp?loc=7-4-0#online

SAND2012-7525
Unlimited Release
Printed September 2012

Revisiting Historic Numerical Analyses of the Waste Isolation Pilot Plant (WIPP) Rooms B and D *in-situ* Experiments Regarding Thermal/Structural Response

Jonathan Scott Rath and J. Guadalupe Argüello

Computational Structural Mechanics and Applications, Org. 01525
Sandia National Laboratories
P.O. Box 5800
Albuquerque, New Mexico 87185-MS-0828

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.

ACKNOWLEDGMENTS

The authors acknowledge James E. Bean for his technical review and editorial contribution to this report. This work was supported by the U.S. Department of Energy (DOE), Office of Nuclear Energy (NE), Fuel Cycle Research and Development (FCR&D) Program.

CONTENTS

FIGURES

TABLES

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:

$$\sigma_{ij,j} + \rho b_j = \rho a_j \qquad \textbf{(2-1)}$$

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

$$\sigma_{ij,j} + f_i = 0 \qquad \textbf{(2-2)}$$

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

$$e_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i} + u_{k,j}u_{k,i}\right) \qquad \textbf{(2-3)}$$

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, $\dot{e}^c_{ij}$, that is highly temperature-dependent. Its overall strain rate can be characterized by the equation:

$$\dot{e}_{ij} = -\frac{\nu}{E}\dot{\sigma}_{kk}\delta_{ij} + \frac{1+\nu}{E}\dot{\sigma}_{ij} + \dot{e}^c_{ij} + 3\alpha\dot{T}\delta_{ij} \qquad \textbf{(2-4)}$$

where ν is the Poisson's ratio, E is Young's Modulus, T is temperature (Kelvin), α is the coefficient of linear thermal expansion, and δ_{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)

$$\dot{T} = \left(k/(\dot{c_p} \cdot \rho)\right)\nabla T \qquad \textbf{(2-5)}$$

where k, c_p, and ρ, are the thermal conductivity, specific heat capacity at constant pressure, and density, respectively, and 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.

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

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.

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

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

$$\dot{\varepsilon}_{s_3} = \left(B_1 e^{-Q_1/RT} + B_2 e^{-Q_2/RT} \right) \sinh\left[q \left(\frac{\sigma_{eq} - \sigma_0}{G} \right) \right] H\left(\sigma_{eq} - \sigma_0 \right) \qquad \textbf{(2-9)}$$

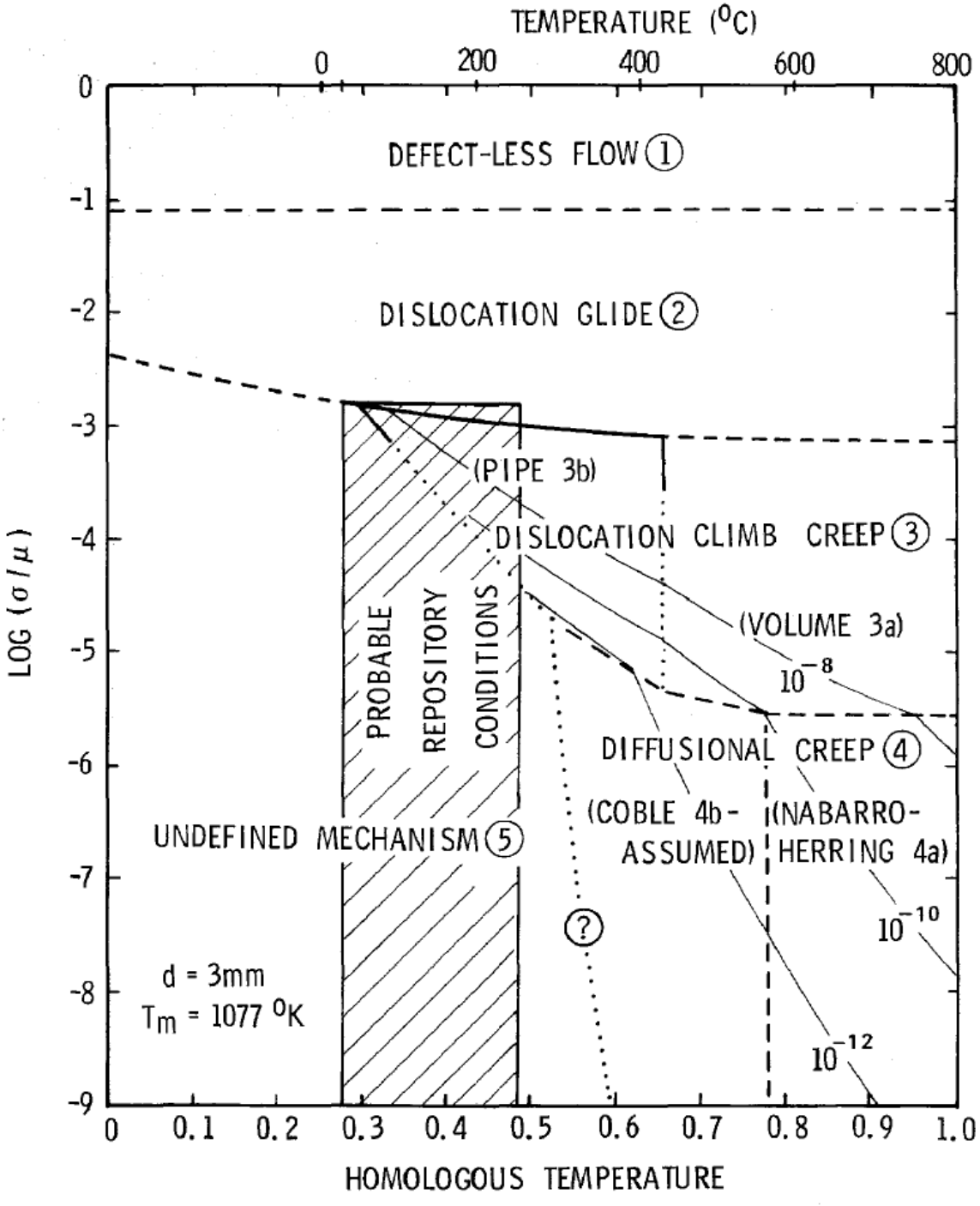


Figure 2-1 Deformation Mechanism Map for Salt (Munson, 1979)

where:

σ_{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
σ_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 σ_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 σ_1 and σ_3 respectively ($\sigma_1 \geq \sigma_2 \geq \sigma_3$). Alternatively, the Tresca stress may be written as a function of the Lode angle ψ and the second invariant J_2 of the deviatoric stress tensor **s** (whose components are s_{ij}).

$$\sigma_{eq} = \sigma_1 - \sigma_3 = 2\cos\psi\sqrt{J_2} \qquad \textbf{(2-10)}$$

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

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

$$J_2 = \frac{1}{2}s_{ij}s_{ij} \qquad \textbf{(2-12)}$$

$$J_3 = \frac{1}{3}s_{ij}s_{jk}s_{ki} \qquad \textbf{(2-13)}$$

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).

$$\dot{\varepsilon}_{eq} = F\dot{\varepsilon}_s \qquad \textbf{(2-14)}$$

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).

$$F = \begin{cases} \exp\left[\Delta\left(1-\dfrac{\zeta}{\varepsilon_t^f}\right)^2\right] & \zeta < \varepsilon_t^f \quad \text{Transient Branch} \\ 1 & \zeta = \varepsilon_t^f \quad \text{Equilibrium Branch} \\ \exp\left[-\delta\left(1-\dfrac{\zeta}{\varepsilon_t^f}\right)^2\right] & \zeta > \varepsilon_t^f \quad \text{Recovery Branch} \end{cases} \qquad \textbf{(2-15)}$$

The choice of the particular branch depends on the transient strain limit, ε_t^f, and the internal variable, ζ. The transient strain limit is defined by Eq. (2-16) where K_0, *c*, and *m* are material parameters, *T* is the absolute temperature, and *G* is the shear modulus.

$$\varepsilon_t^f = K_0 e^{cT}\left(\frac{\sigma_{eq}}{G}\right)^m \qquad \textbf{(2-16)}$$

The internal variable, ζ, appearing in the calculation of the function, *F*, is obtained by integration of the evolution equation

$$\dot{\zeta} = (F-1)\dot{\varepsilon}_s \qquad \textbf{(2-17)}$$

Δ and δ, 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 α, β, α_r, and β_r are material parameters. Typically the recovery parameter δ is taken to be constant (*i.e.*, $\delta = \alpha_r$).

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

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

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

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

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

$$\dot{e}_{ij}^{c} = \dot{\varepsilon}_{eq} \frac{\partial \sigma_{eq}}{\partial \sigma_{ij}} = \dot{\varepsilon}_{eq} N_{ij} \qquad \textbf{(2-21)}$$

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.

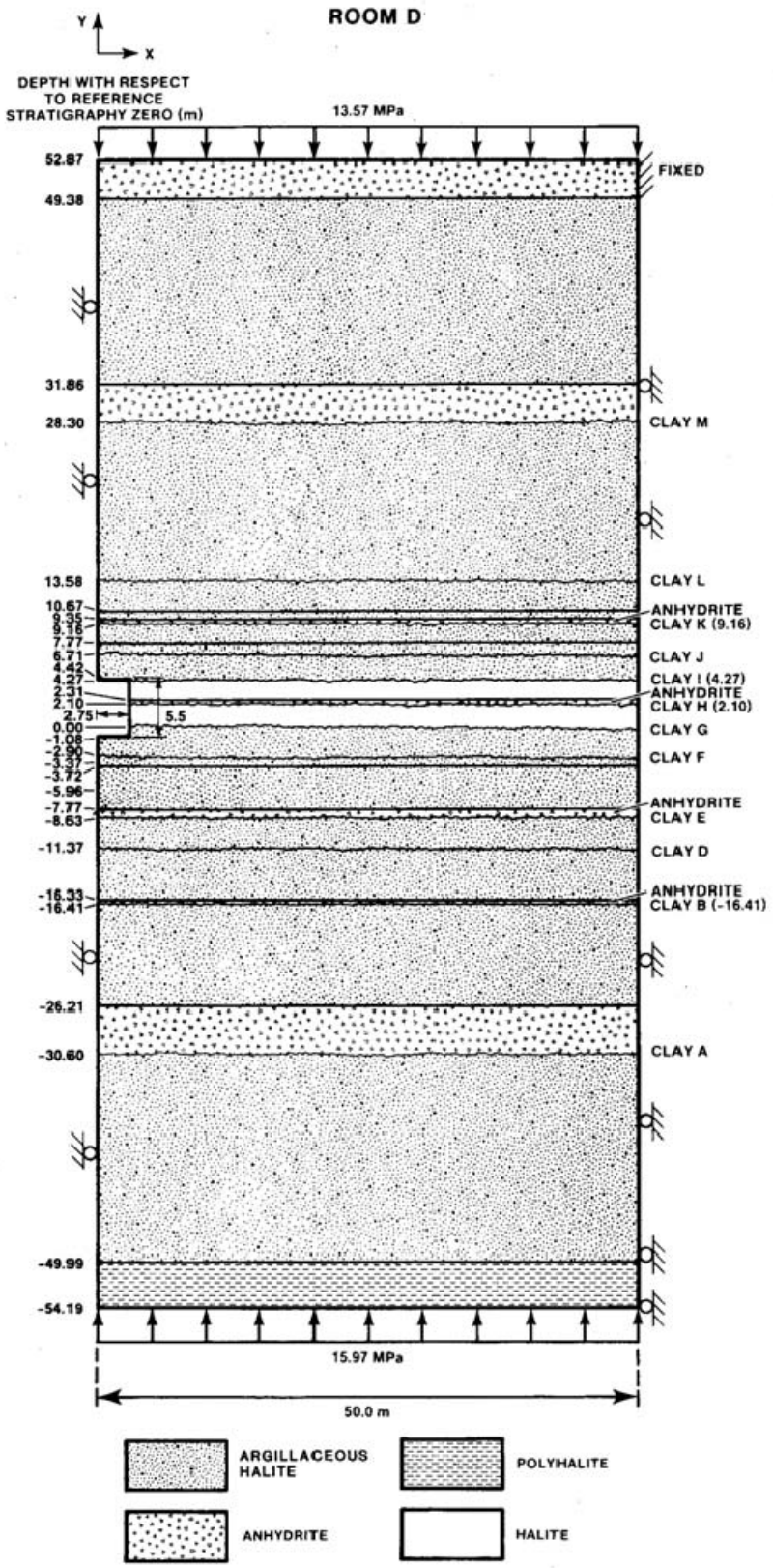


Figure 3-1 Local stratigraphy around and model of Room D.

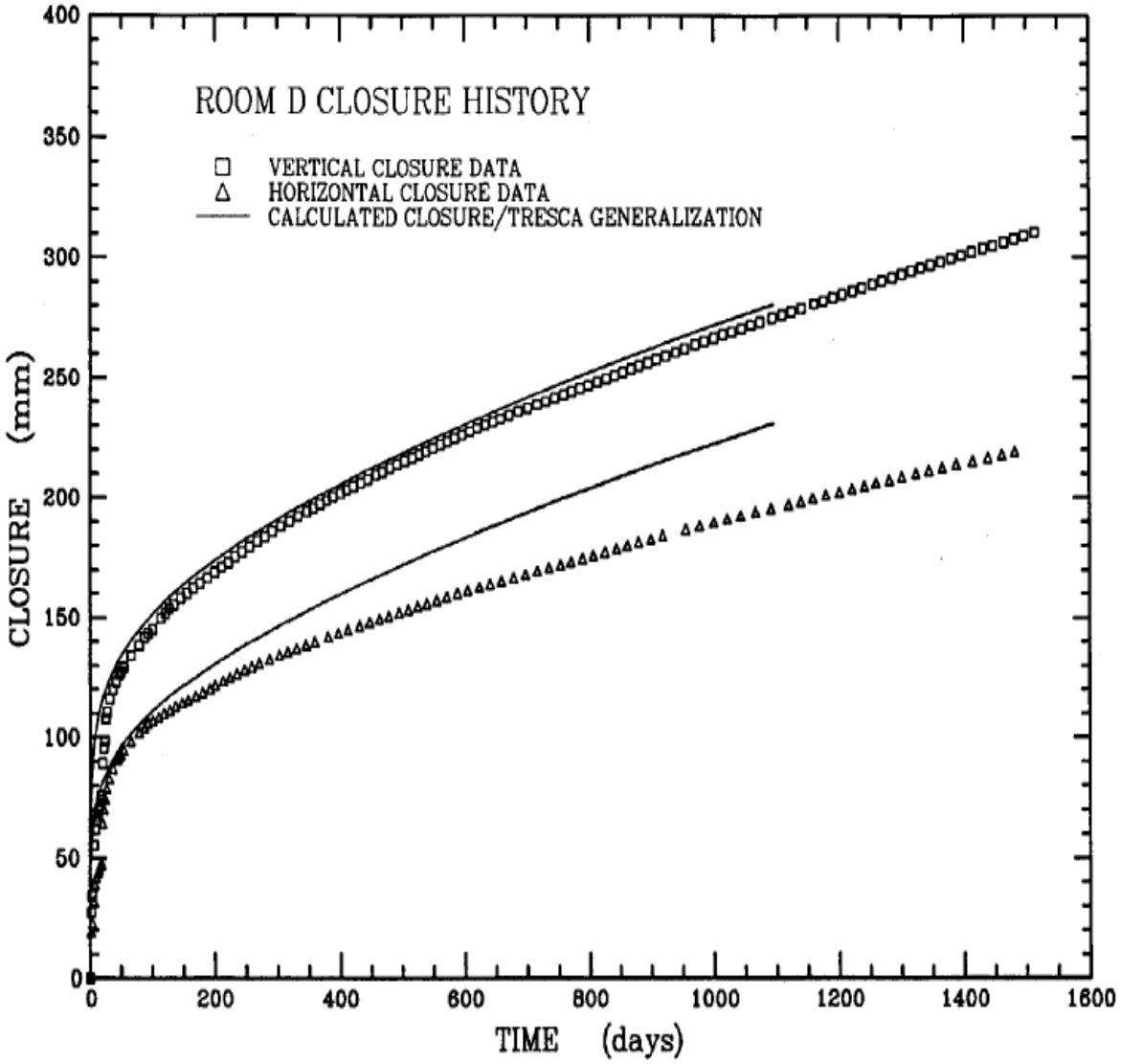


Figure 3-2 Comparison of calculated (SPECTROM-32) and measured in-situ Room D closures from historical calculation (Munson et al. 1989).

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, μ, 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

far-field boundary placed sufficiently far into the salt. 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.

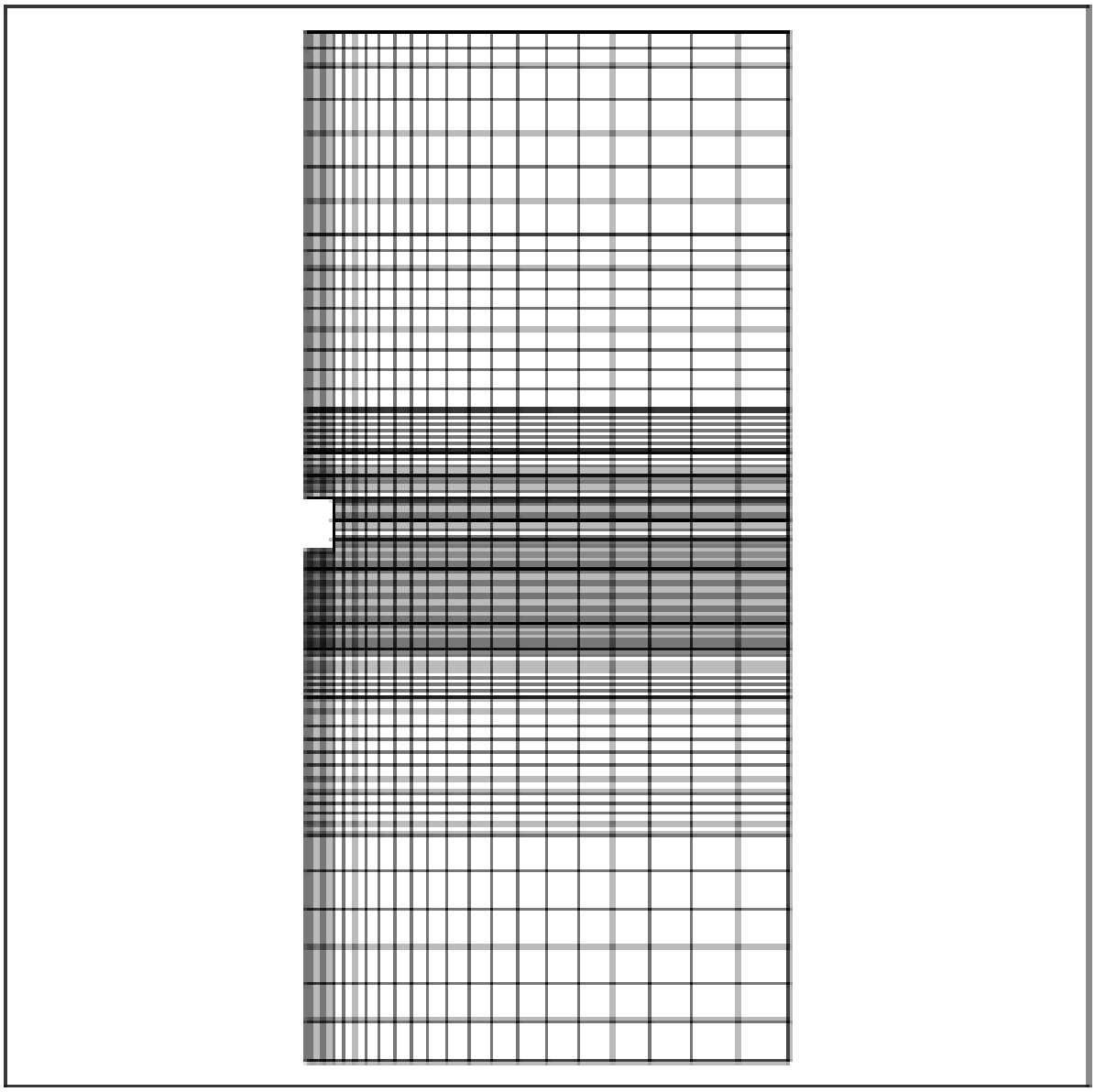


Figure 3-3 Overall mesh used for the SIERRA Mechanics Room D simulation.

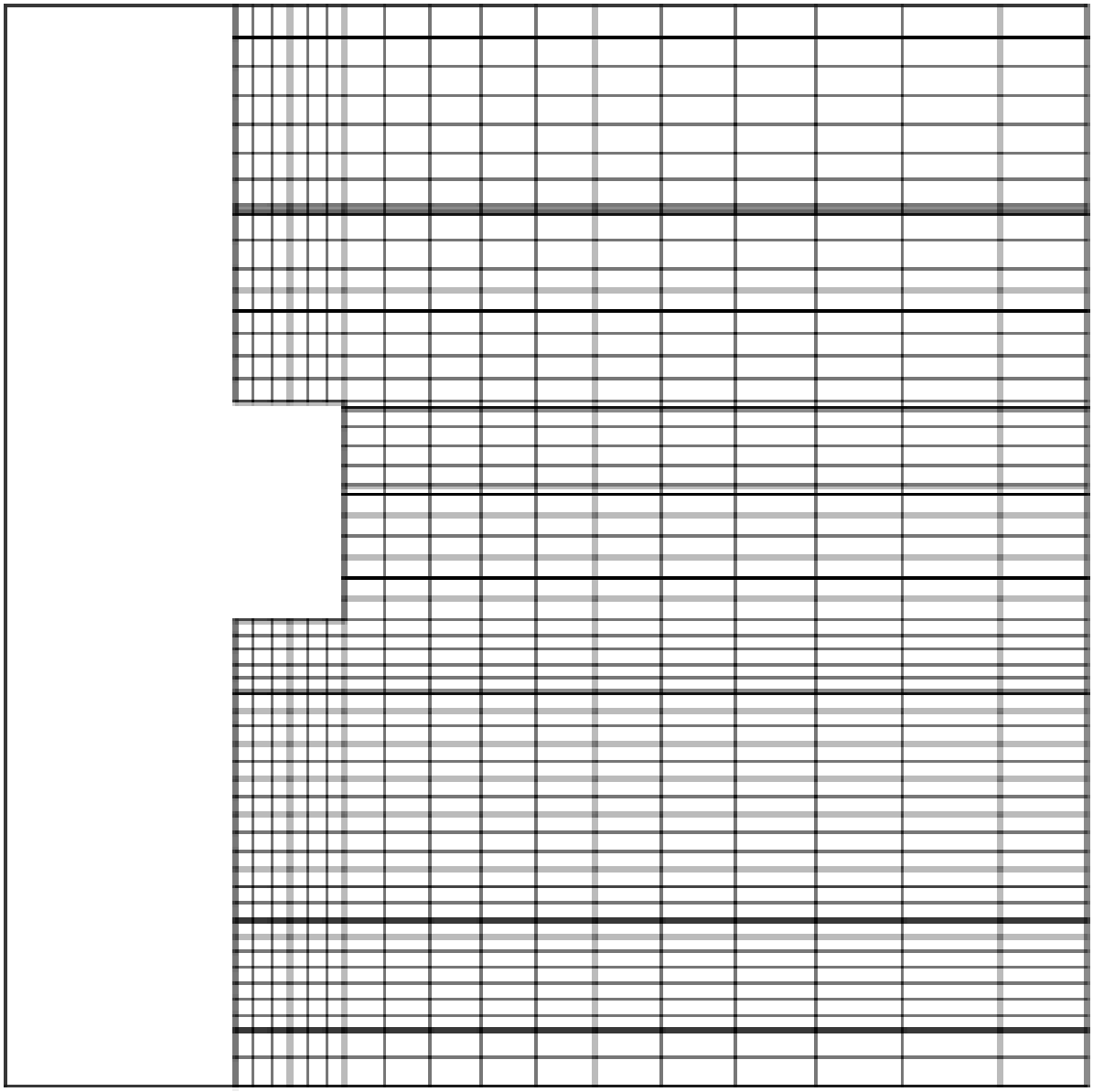


Figure 3-4 Close-up of mesh in the vicinity of the room used for the SIERRA Mechanics Room D simulation.

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

	Parameters		Units	Salt	Arg. Salt
Elastic Properties	Shear modulus	G	MPa	12,400	12,400
	Young's modulus	E	MPa	31,000	31,000
	Poisson's ratio	ν	–	0.25	0.25
Salt Creep Properties	Structure Factors	A_1	s^{-1}	8.386×10^{22}	1.407×10^{23}
		B_1		6.086×10^{6}	8.998×10^{6}
		A_2		9.672×10^{12}	1.314×10^{13}
		B_2		3.034×10^{-2}	4.289×10^{-2}
	Activation energies	Q_1	cal/mole	25,000	25,000
		Q_2	cal/mole	10,000	10,000
	Universal gas constant	R	cal/mol-K	1.987	1.987
	Absolute temperature	T	K	300	300
	Stress exponents	n_1	–	5.5	5.5
		n_2		5.0	5.0
	Stress limit of the dislocation slip mechanism	σ_0	MPa	20.57	20.57
	Stress constant	q	–	5,335	5,335
	Transient strain limit constants	M	–	3.0	3.0
		K_0	–	6.275×10^{5}	2.470×10^{6}
		c	K^{-1}	9.198×10^{-3}	9.198×10^{-3}
	Constants for work-hardening parameter	α	–	-17.37	-14.96
		β	–	-7.738	-7.738
	Recovery parameter	δ	–	0.58	0.58

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.

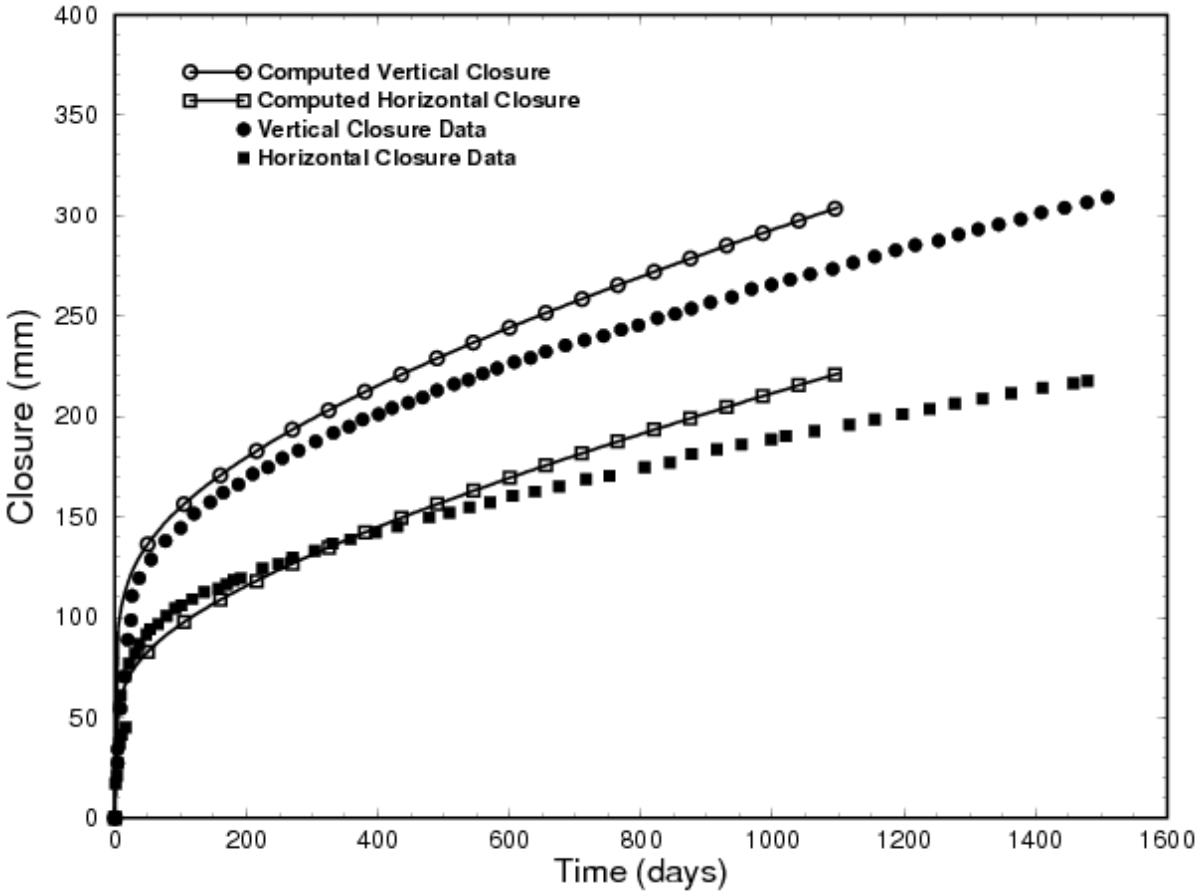


Figure 3-5 Comparison of computed (SIERRA Mechanics) and measured in-situ Room D closure response.

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

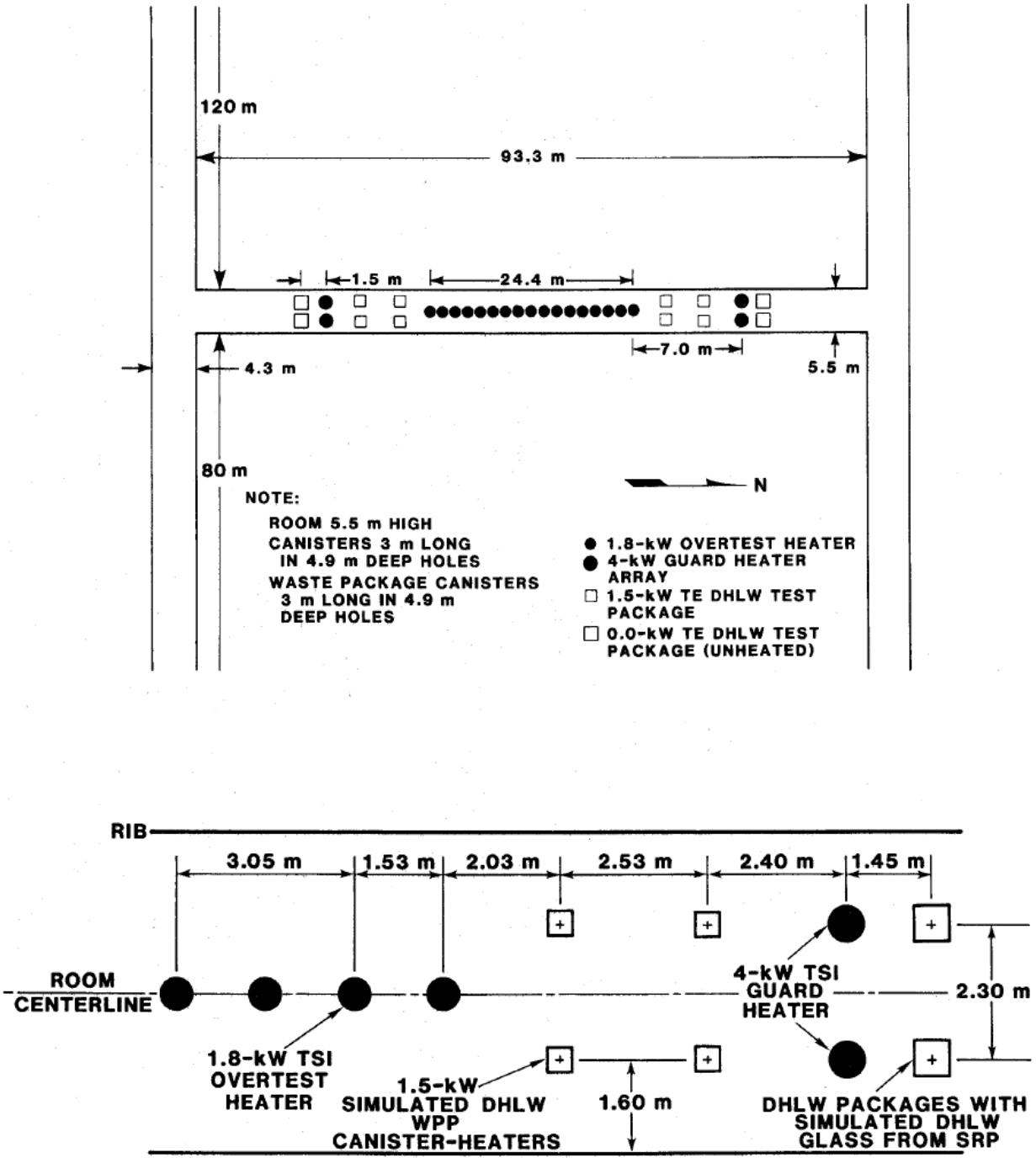


Figure 4-1 Plan View of WIPP Room B and Heater Emplacement Locations.

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.

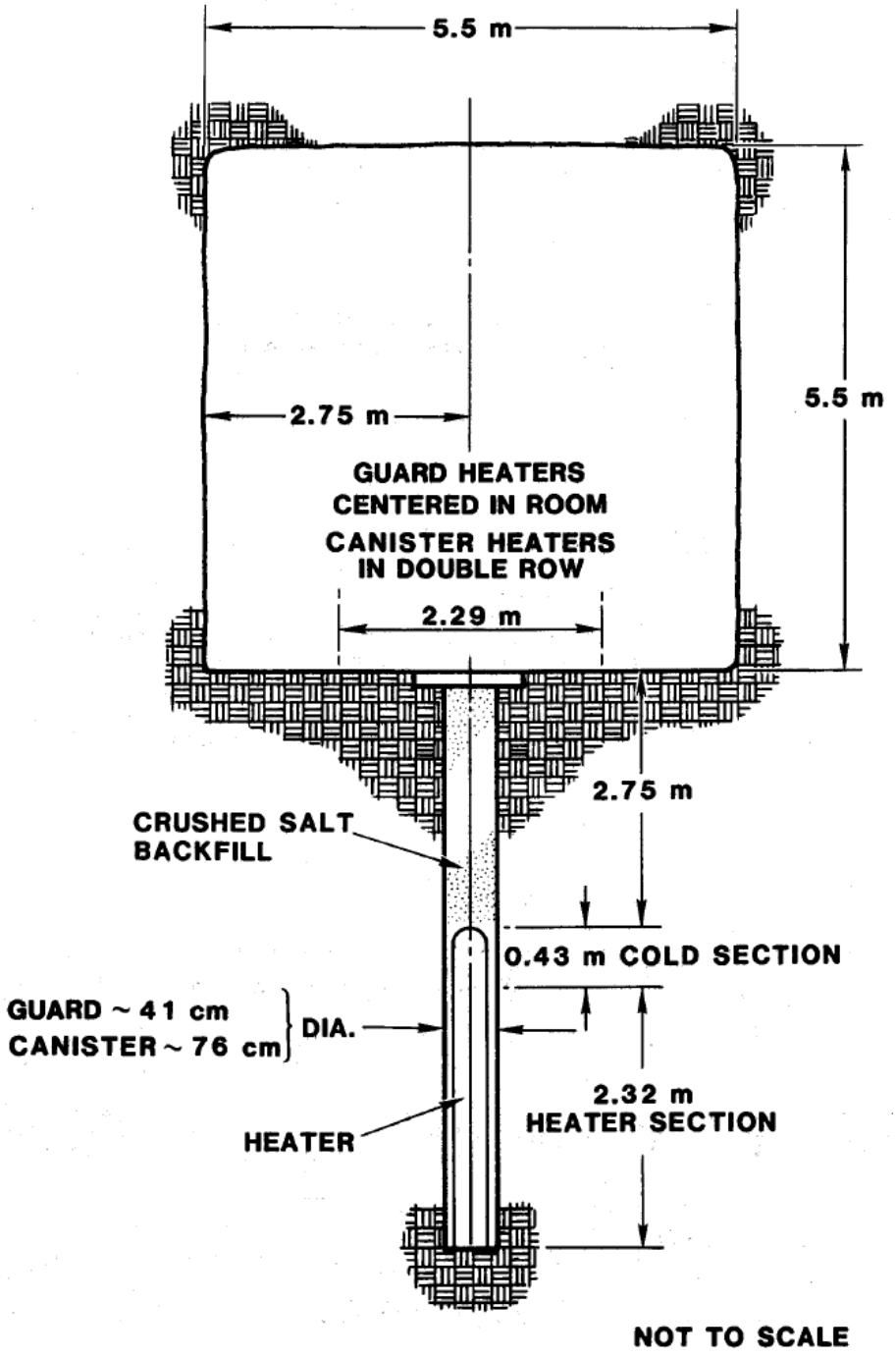


Figure 4-2 Details of Canister Emplacement for the WIPP Room B

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 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 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.

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/m^2 condition on the symmetry plane, only half of this load or 228 W/m^2 was applied to the thermal finite element model. A thirty year half-life was simulated as a decaying exponential so the therma1 load applied along the length of the heat source had the form

$$q = 228 * \exp(-7\ 327 \times 10^{-10} * t) \qquad (4\text{-}1)$$

where q is the thermal load in W/m^2 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

$$\lambda = \lambda_{300} (300/T)^{\gamma} \qquad (4\text{-}2)$$

where λ is the thermal conductivity, T is the absolute temperature in Kelvin (K), and λ_{300} and γ 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 4-1 Thermal Properties used in Room B Thermal Simulations Using Aria

Material	Density, ρ (kg/m^3)	Specific Heat, C_p (J/kg/K)	Thermal Conductivity Parameters	
			λ_{300} (W/m/K)	γ
Halite	2300.0	860.0	5.0	1.14

ETM	1.0	1000.0	50.0	0.0

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:

$$q' \cdot n = h \cdot (T - 300) \qquad (4\text{-}3)$$

where $\boldsymbol{q'}$ is the thermal flux vector, $\boldsymbol{n}$ is the outward normal unit vector, $\boldsymbol{h}$ is the convective heat transfer coefficient, and $\boldsymbol{T}$ 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 $W/m^2/K$) 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 $W/m^2/K$ 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.

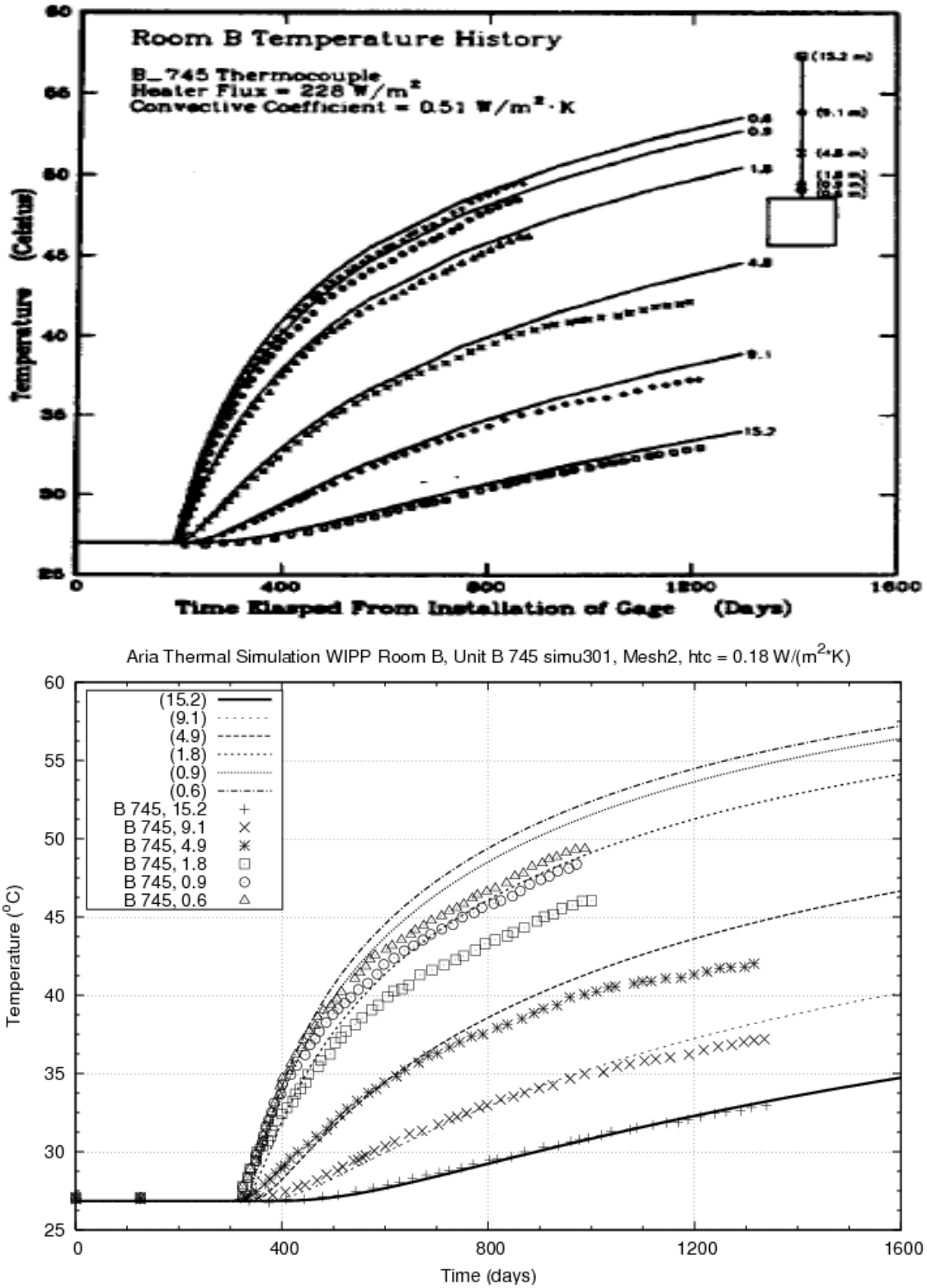


Figure 4-3 SPECTROM-41 Thermal Simulation (above) and Aria Thermal Simulation (below) Compared with Room B Thermocouple B_745 locations

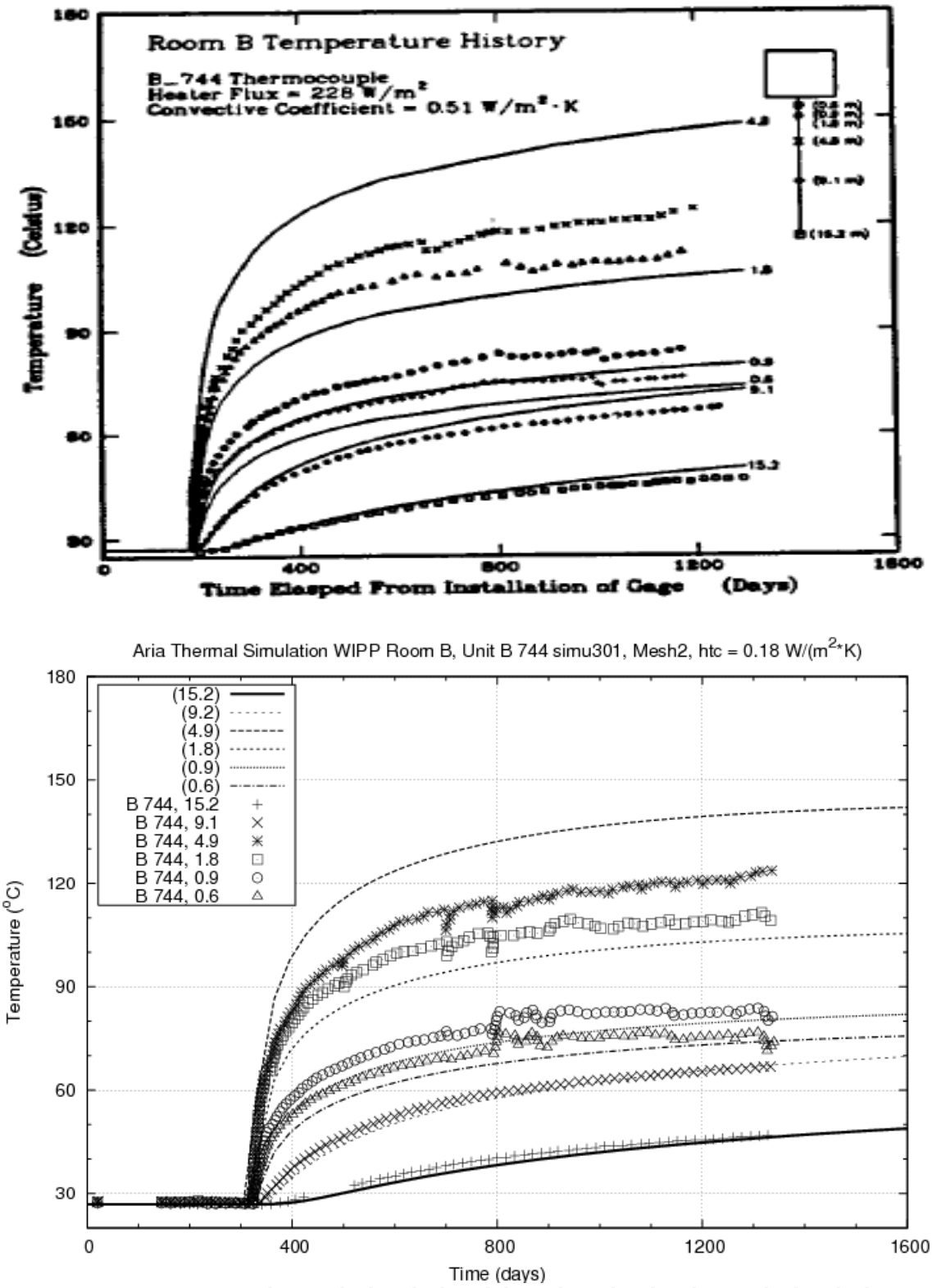


Figure 4-4 SPECTROM-41 Thermal Simulation (above) and Aria Thermal Simulation (below) Compared with Room B Thermocouple B_744 locations.

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).

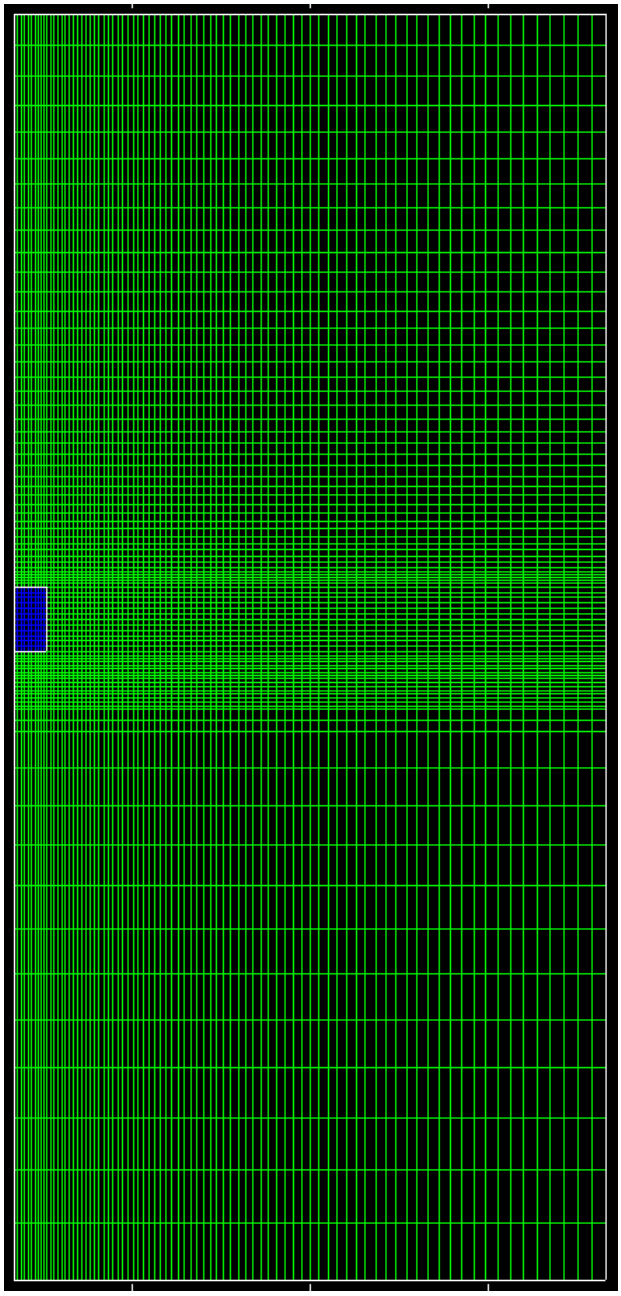


Figure 4-5 Aria Finite Element Mesh Plane View (XY-plane) showing Halite Material (green) and "Equivalent Thermal Material" (blue).

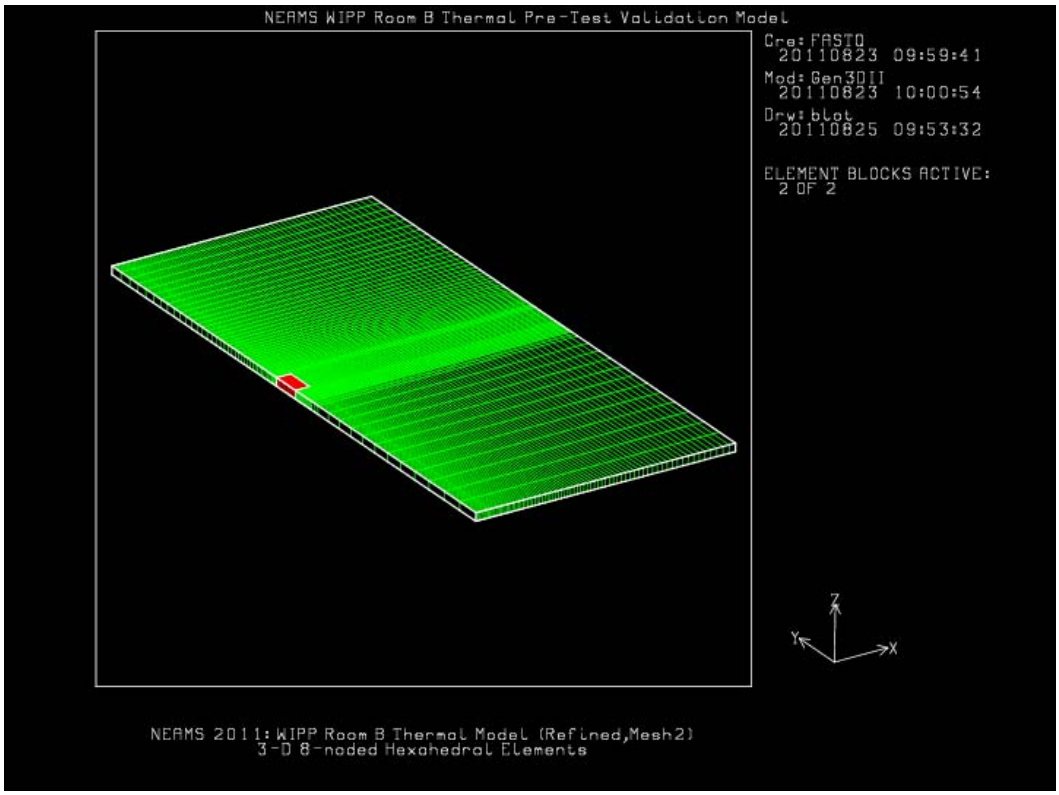


Figure 4-6 Aria Three Dimensional 8-node Hexahedral Finite Element Mesh used in Thermal simulations

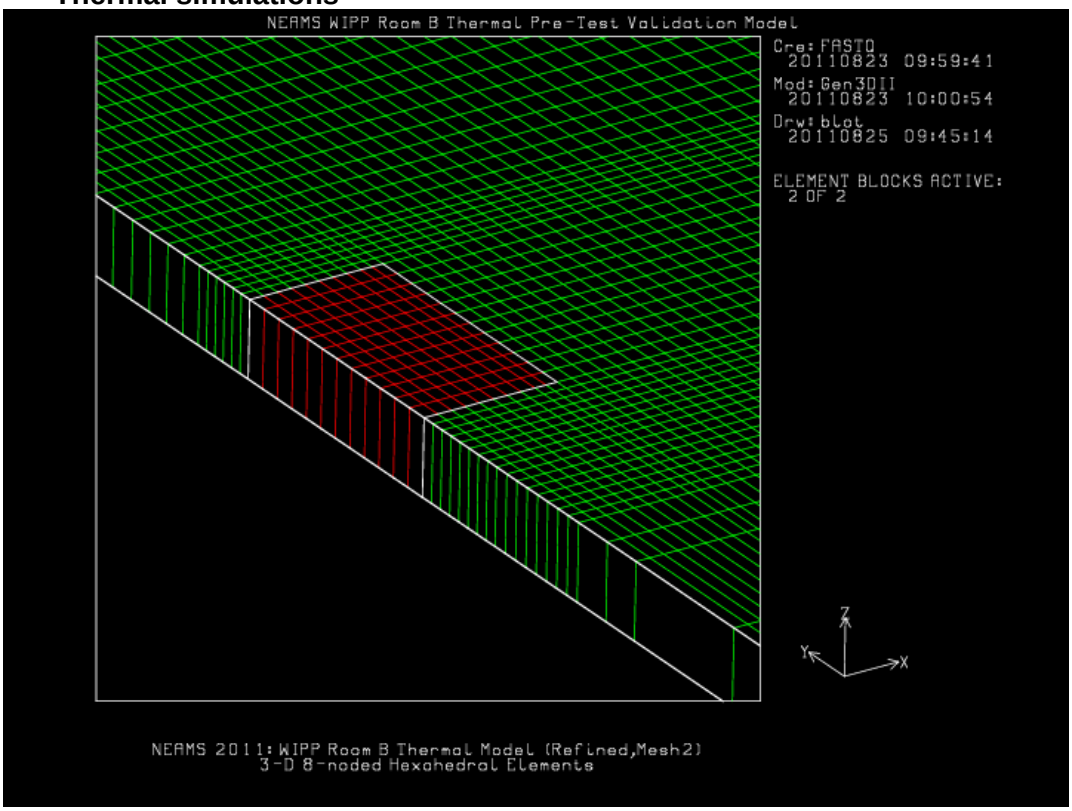


Figure 4-7 Zoomed in Detail of Aria 3D Finite Element Mesh Near Room B Location (shown in red)

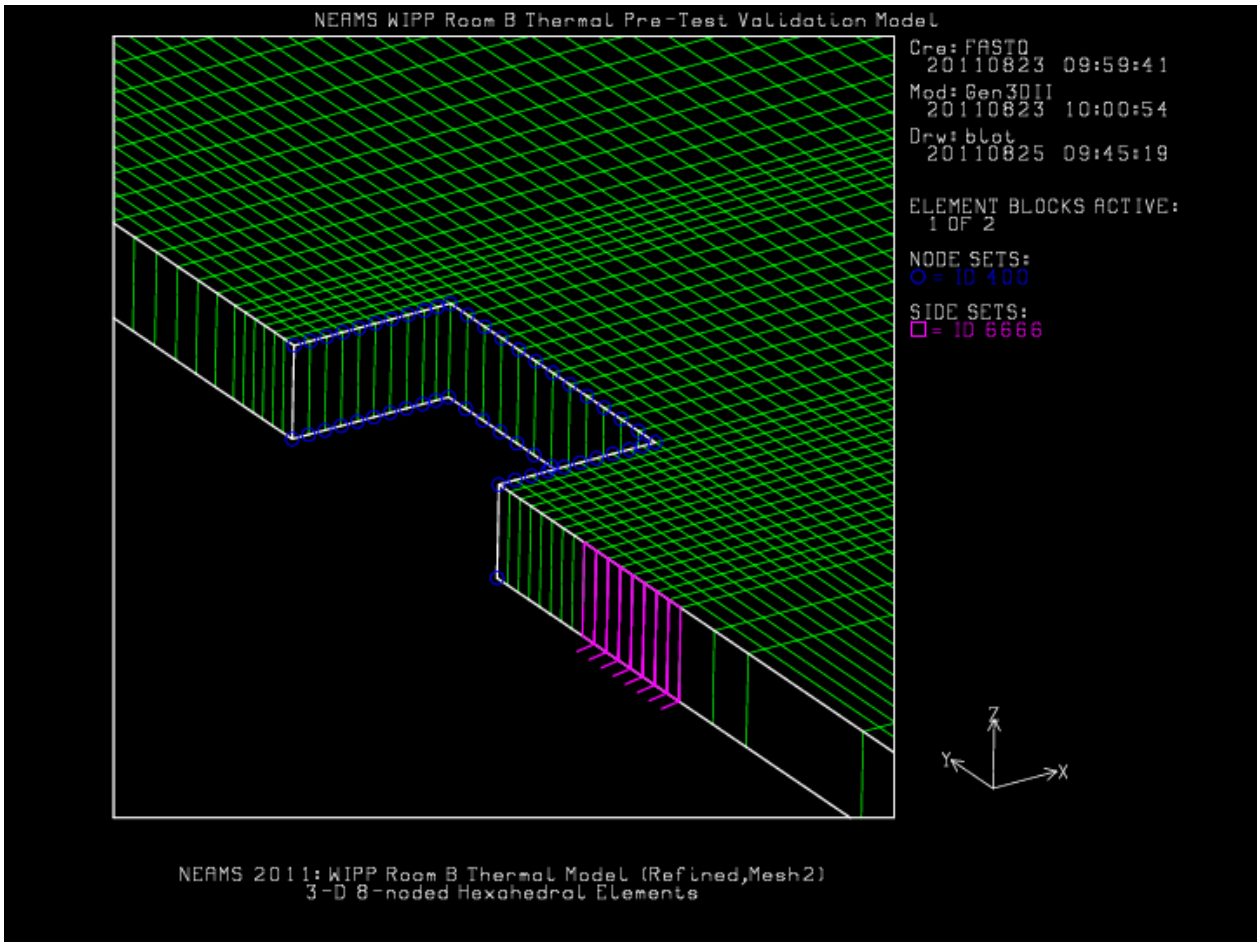


Figure 4-8 Aria finite element model location of heat source and thermal convection boundary.

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 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.

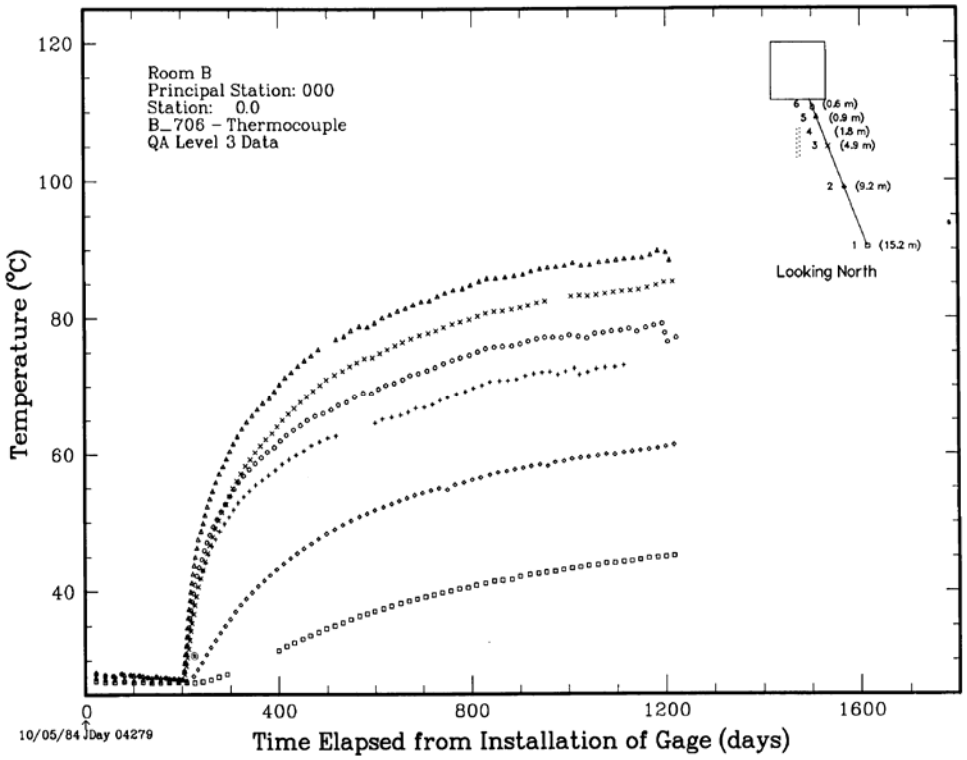


Figure 5.3.1d. Thermocouple Unit B 706

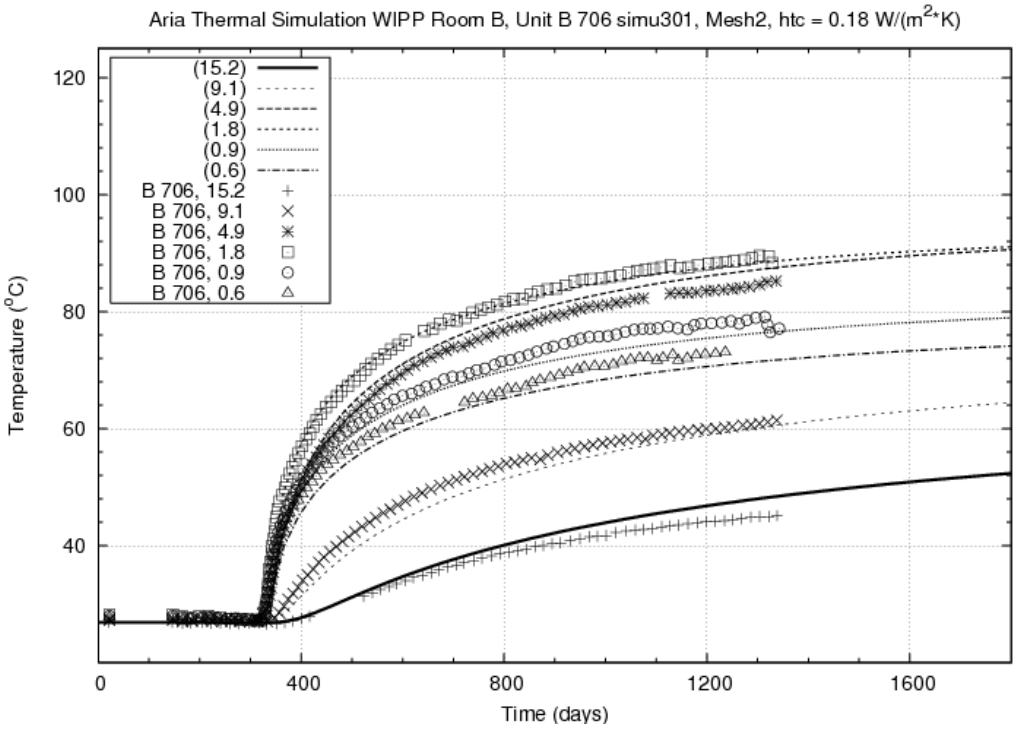
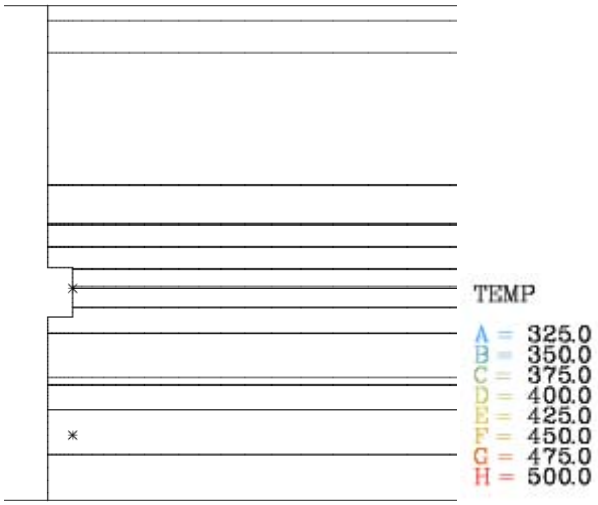


Figure 4-9 Measured temperatures at thermocouple Unit B 706 (top) and comparison of Aria predicted temperatures with measured temperatures (bottom).

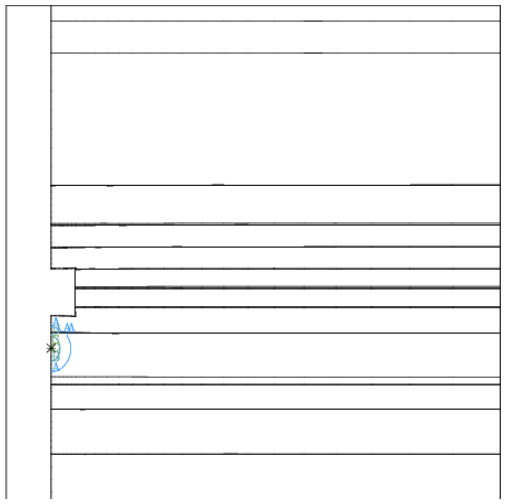
Table 4-2 Tabulated Comparisons of Simulated Temperatures to Thermocouple Temperatures at gage B_706 at 1200 years.

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

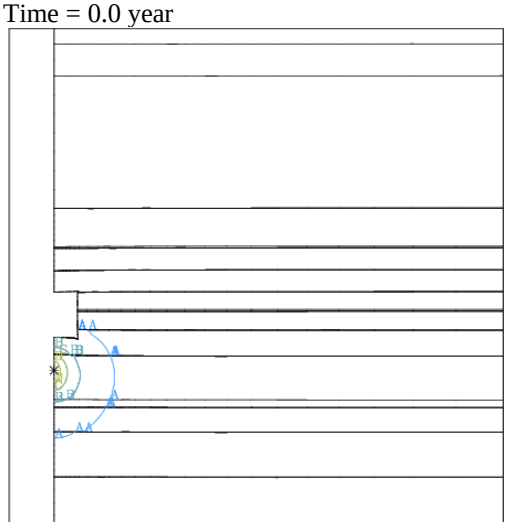
In general, the comparison of temperatures predicted by Aria and compared to the temperatures measured at thermocouple locations at Unit B 706, shown in Figure 4-9, are reasonable with respect to the uncertainty of the equivalent thermal material model property values. One metric for measuring the quality 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.



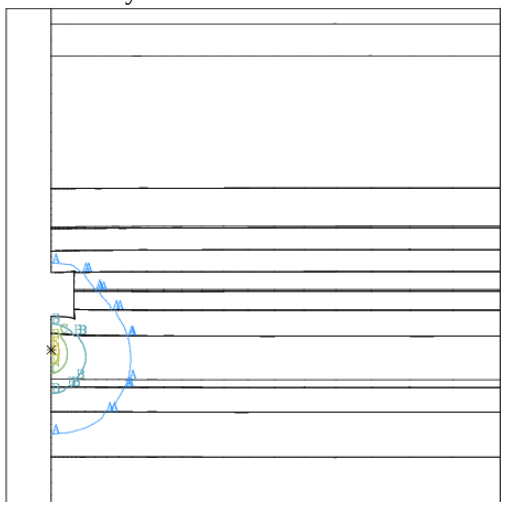
Time = 0.0 year



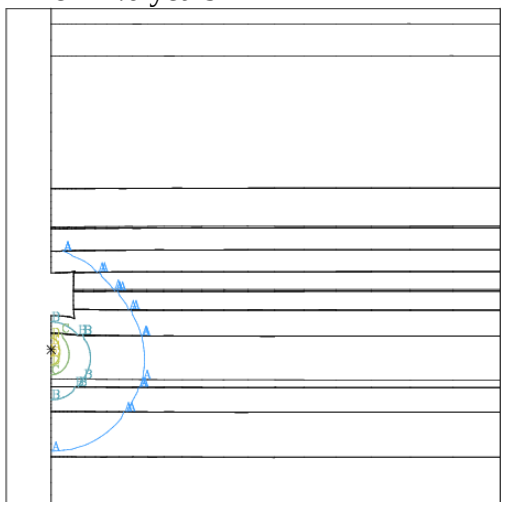
Time = 1.0 year



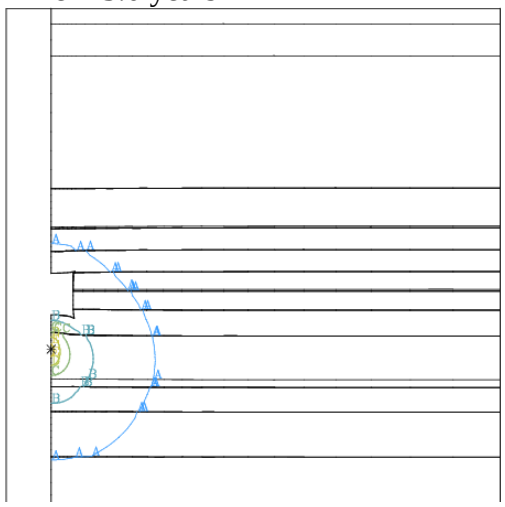
Time = 2.0 years



Time = 3.0 years

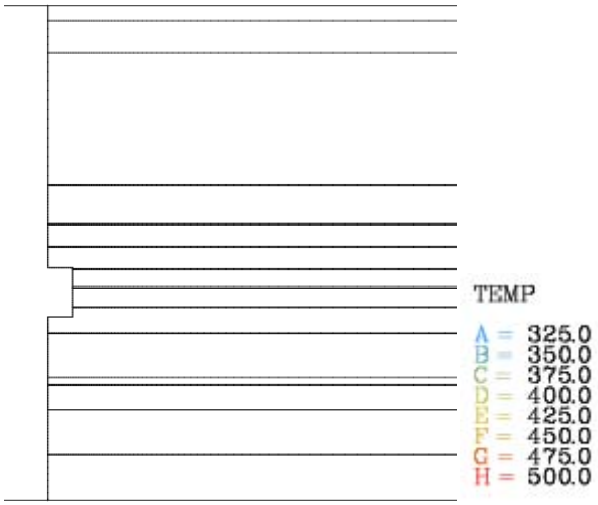


Time = 4.0 years

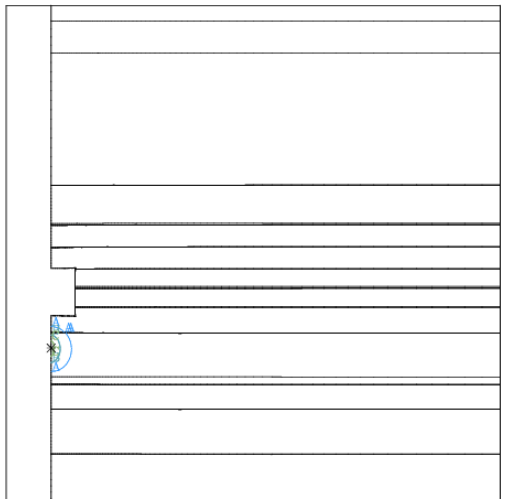


Time = 5.0 years

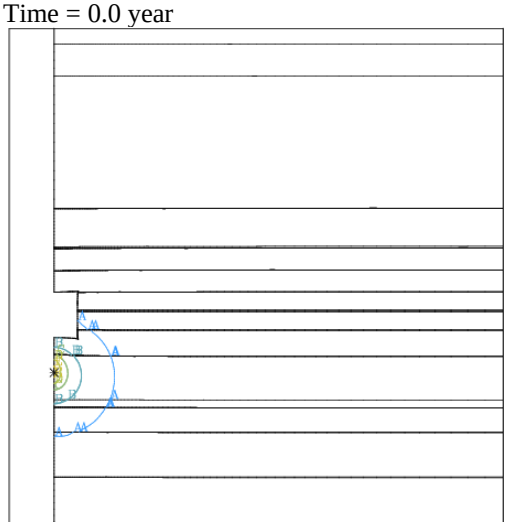
Figure 4-10 Coarse Thermal Mesh Computed Temperature Contours Drawn over Coarse Structural Deformed Mesh at Time = 0, 1, 2, 3, 4, and 5 years.



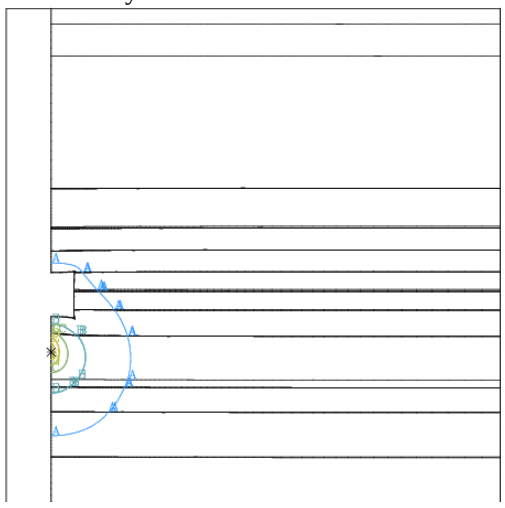
Time = 0.0 year



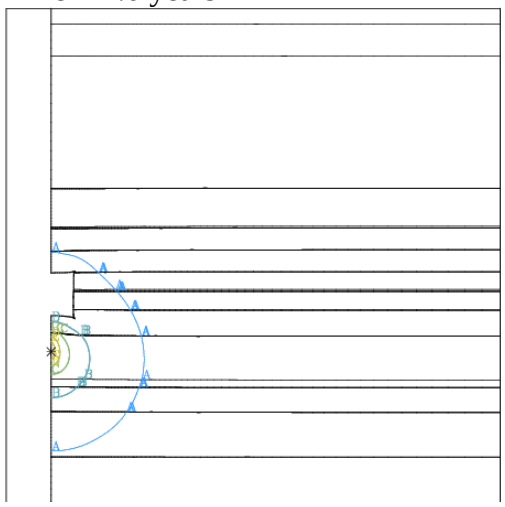
Time = 1.0 year



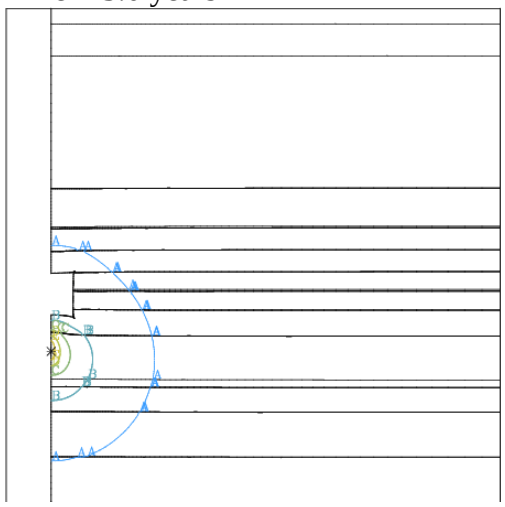
Time = 2.0 years



Time = 3.0 years



Time = 4.0 years



Time = 5.0 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). Tractions 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 $\Delta Z_{\text{element}}$ = 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).

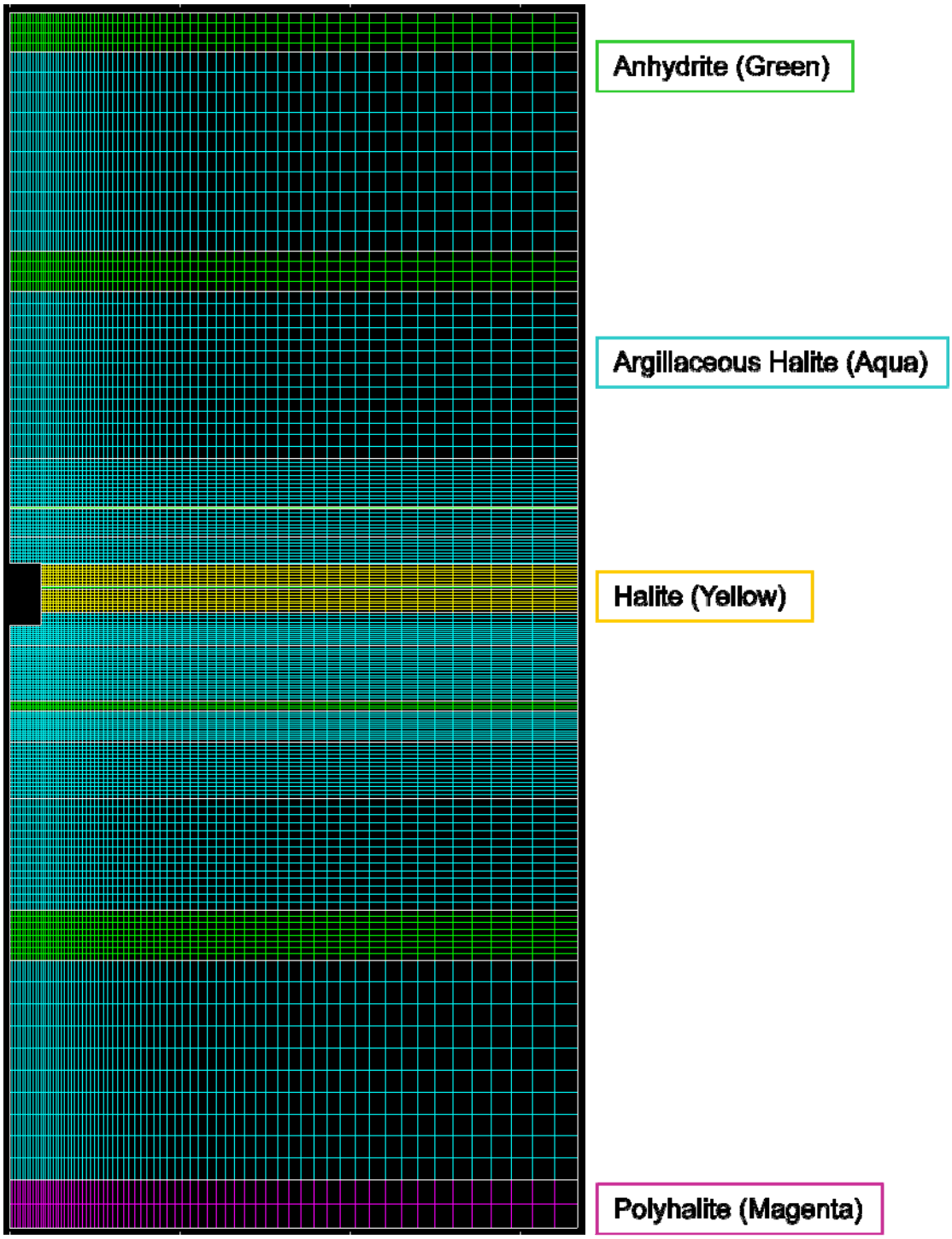


Figure 4-12 Heated Room Structural Model Finite Element Mesh

Figure 4-13 Heated Room Structural Finite Element Model, Zoom view.

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

$$\sqrt{J_2'} = C - aJ_1 \qquad \text{(4-4)}$$

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

$$\bar{\sigma} = \sqrt{3}C + 3\sqrt{3}aP \quad (4\text{-}5)$$

or

$$\bar{\sigma} = a_0 + a_1 P \quad (4\text{-}6)$$

where $\bar{\sigma}$ is the von Mises or equivalent stress (and $\bar{\sigma} = \sqrt{3}\sqrt{J_2'}$), $\boldsymbol{P}$ is the pressure (negative one third of the trace of the stress tensor), and $\boldsymbol{a_0}$ and $\boldsymbol{a_1}$ 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.*, $\boldsymbol{a_2}$) 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

Creep Parameter	Halite	Argillaceous Halite	Units
Shear Modulus, G	$1.249 \times 10^{+10}$	$1.24 \times 10^{+10}$	Pa
Poisson Ratio, ν	0.2484221834	0.25	1
A_1	$8.386 \times 10^{+22}$	$1.406 \times 10^{+23}$	sec^{-1}
Q_1/R	12581.78158	12581.78	Kelvin
N_1	5.5	5.5	1
B_1	6086000	8993300	sec^{-1}
A_2	$9.672 \times 10^{+12}$	$1.3131 \times 10^{+13}$	sec^{-1}
Q_2/R	5032.71	5032.71	Kelvin
N_2	5	5	1
B_2	0.03034	0.042875	sec^{-1}
σ_0	20570000	20570000	Pa
Q_{lc}	5335	5335	1
M	3	3	1
K_0	627500	2470000	1
C	0.009189	0.009189	$Kelvin^{-1}$
Alpha	-17.37	-14.96	1
Beta	-7.738	-7.738	1
DelatC	0.58	0.58	1
Algorithm Parameter	**Halite**	**Argillaceous Halite**	**Units**
Amult	0.5	0.5	1
Grwfac	1.05	1.05	1
Esptol	0.01	0.01	1
Shkfac	1	1	1
Itype	0	0	1
Angle	0.1	0.1	1

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

Parameter	Anhydrite	Polyhalite	Units
Elastic Modulus, E	$7.51 \times 10^{+10}$	$5.53 \times 10^{+10}$	Pa
Poisson Ratio, ν	0.36	0.36	1
C, Prager-Drucker	$1.35 \times 10^{+6}$	$1.42 \times 10^{+6}$	Pa
a, Prager-Drucker	0.45	0.473	1
a_0, Soil-Crushable Foam	2338268.59	2459512.147	Pa
a_1, Soil Crushable Foam	2.33826859	2.45778096	1

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, α_T as a piecewise linear functions of temperature and strain:

T_{ref} Thermal Strain = 0.0

T_{max} Thermal Strain = $(T_{max} - T_{ref}) * \alpha_T$

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

Table 4-5 Coefficients of Linear Thermal Expansion

Material	Coefficient of Linear Thermal Expansion, α_T [Kelvin^{-1}]
Polyhalite	24.0×10^{-6}
Argillaceous Halite	40.0×10^{-6}
Anhydrite	20.0×10^{-6}
Halite	45.0×10^{-6}

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 μ, 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 μ times the normal stress. A coefficient of friction value, μ = 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.

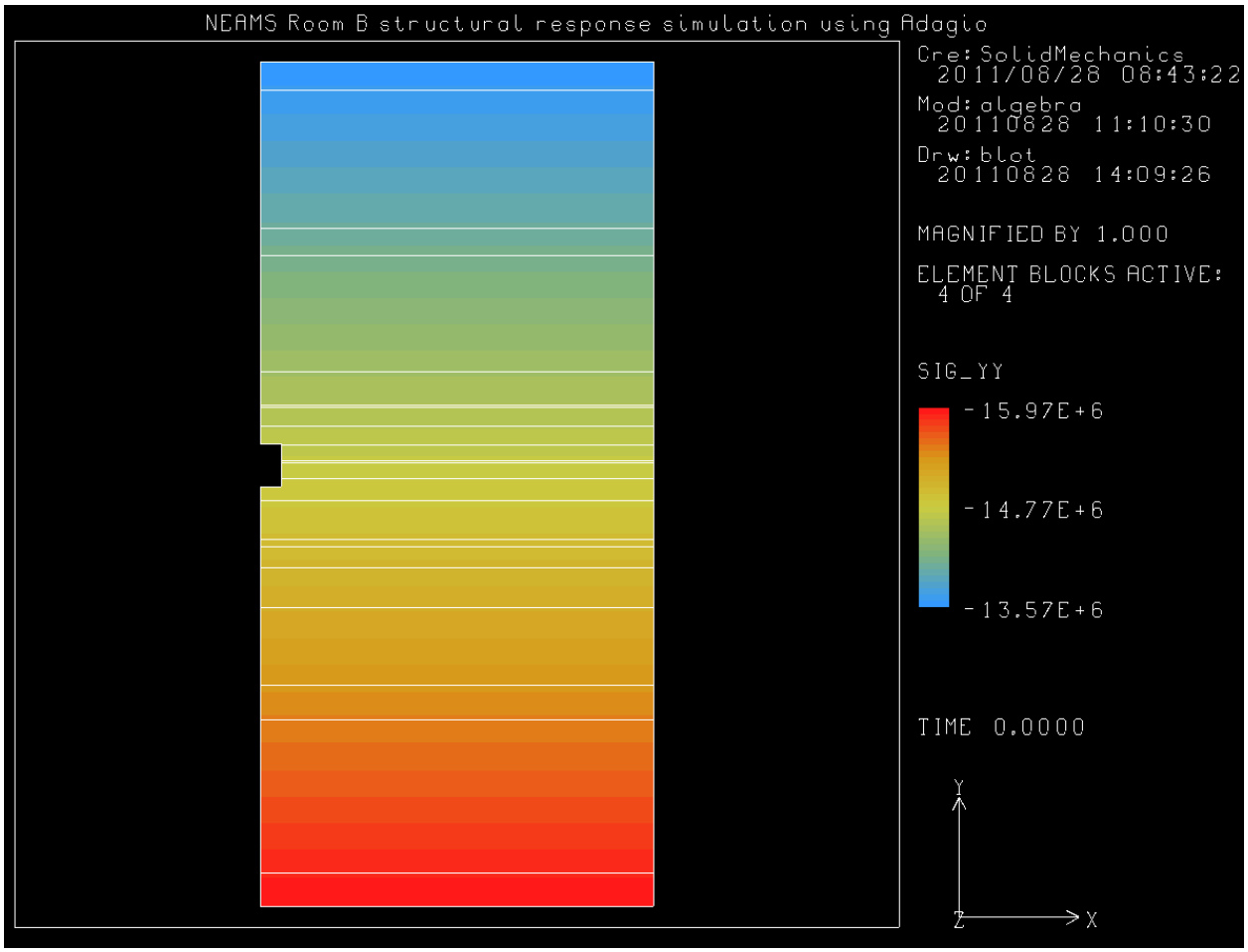


Figure 4-14 Heated Room Initial Stress Condition at Simulation Time t = 0.

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.

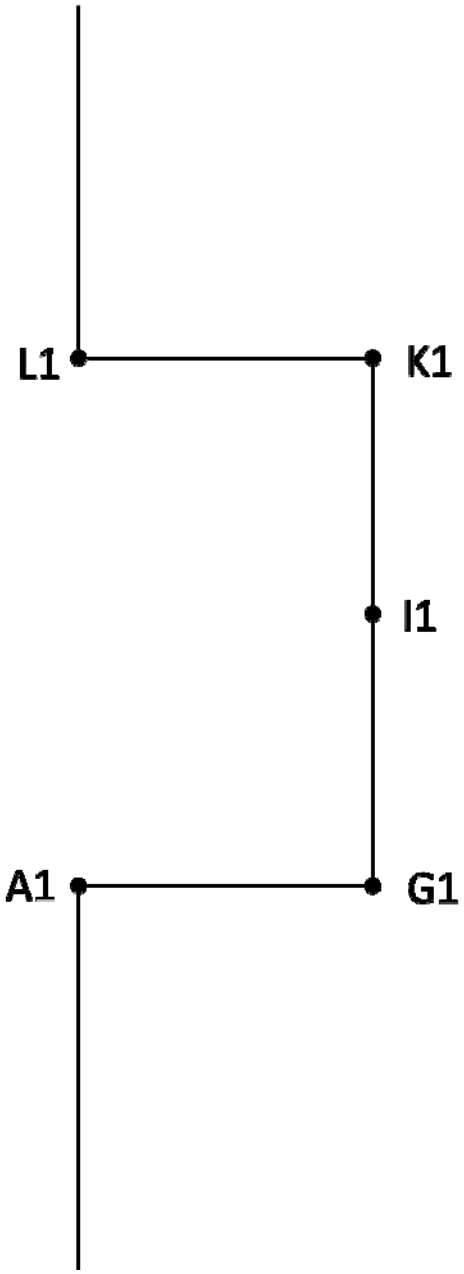


Figure 4-15 Room B Closure Measurement Geometry.

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 place 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.

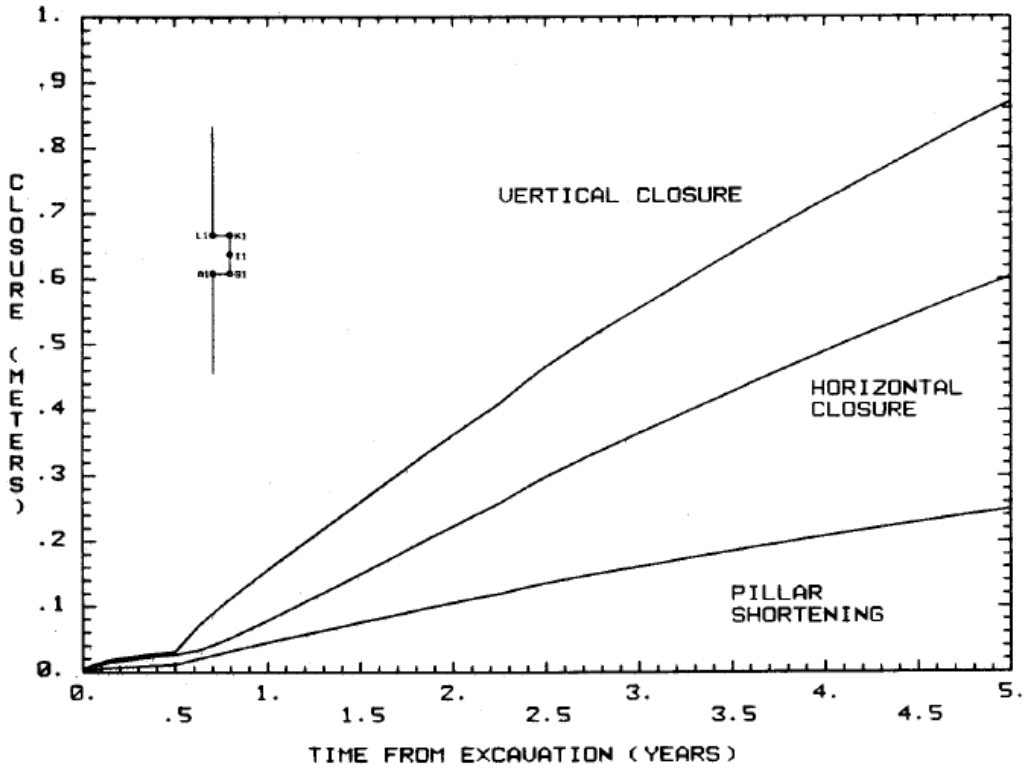


Figure 4-16 Room B Closure Response predicted by a SANCHO two dimensional calculation [9].

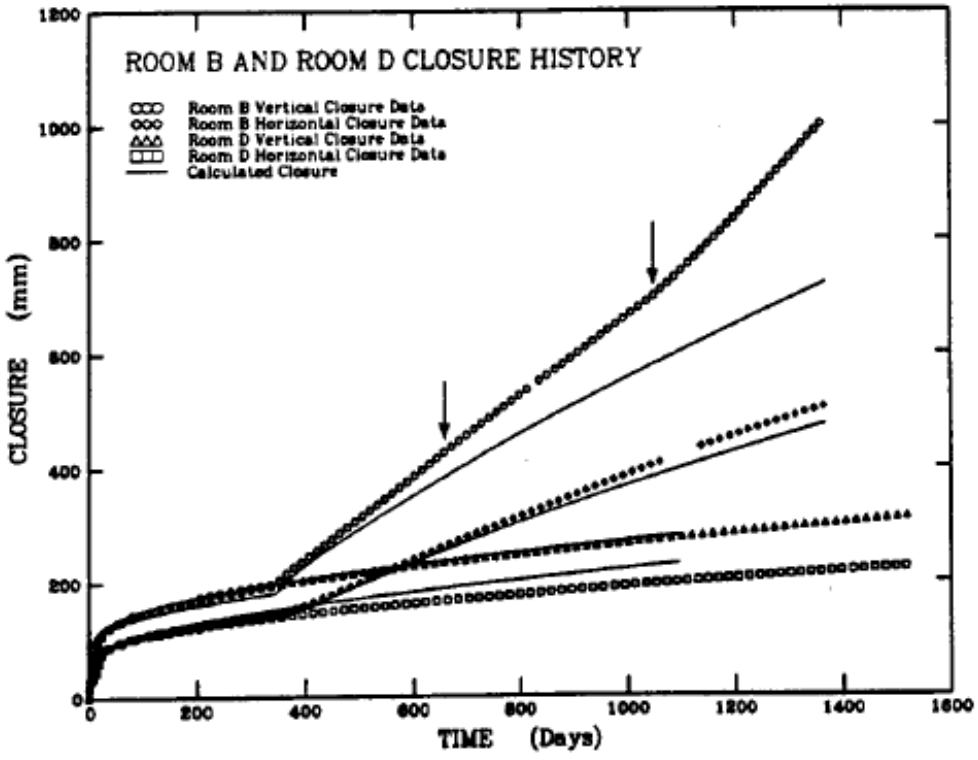


Figure 4-17 Room B Closure Response predicted by SPECTROM-32 and compared with recorded extensometer test data [19].

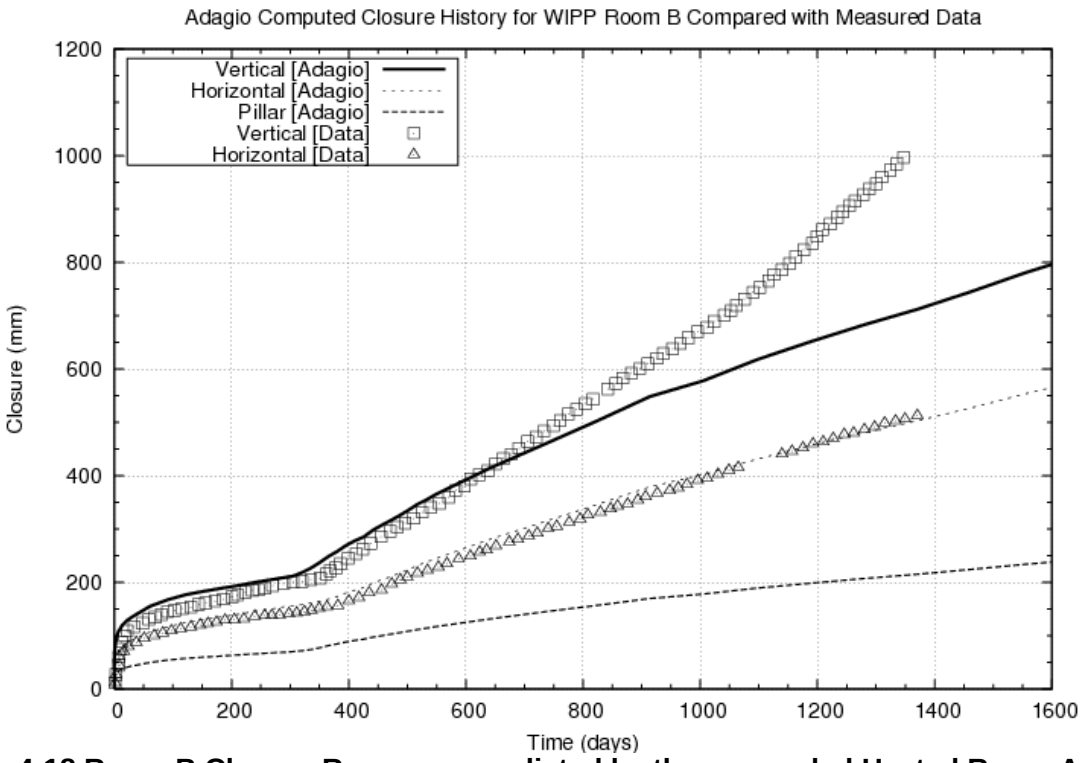


Figure 4-18 Room B Closure Response predicted by the uncoupled Heated Room Adagio simulation and compared to recorded extensometer test data (Coarse Mesh).

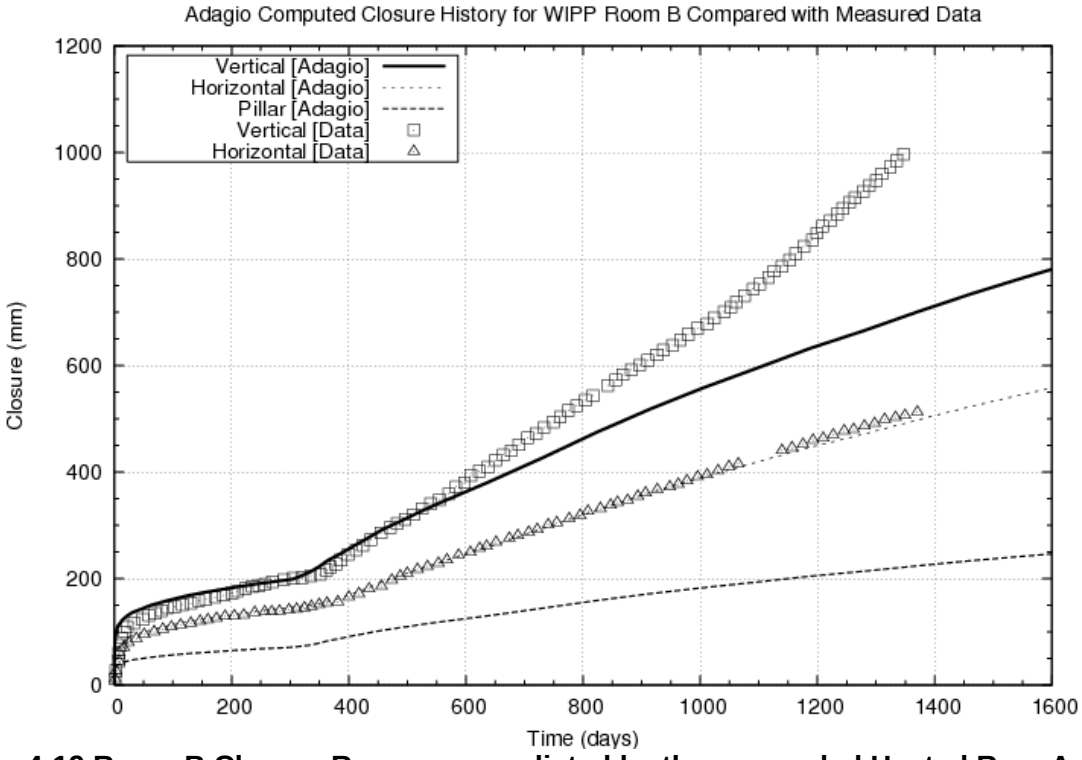


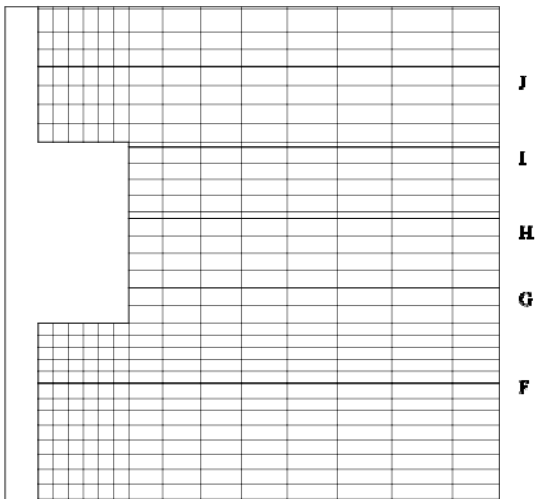
Figure 4-19 Room B Closure Response predicted by the uncoupled Heated Rom Adagio simulation and compared to recorded extensometer test data (Reference Mesh).

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).

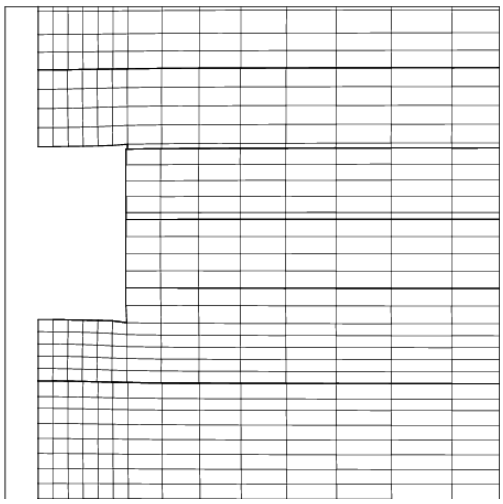
Table 4-6 Computed Heated Room Closure Response compared with Extensometer Data at 1200 days

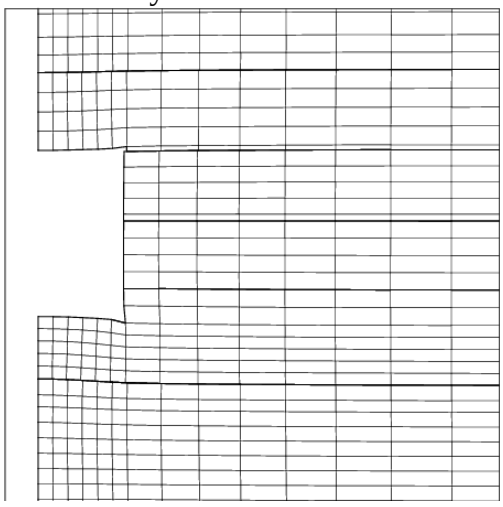
Source	Vertical Closure (m)	Horizontal Closure (m)	Difference Between Experiment and Simulation: Vertical Closure (%)	Difference Between Experiment and Simulation: Horizontal Closure (%)
Test Data	0.85	0.46	N/A	N/A
SANCHO	0.60	0.40	29	15
SPECTROM-32	0.67	0.42	21	11
Adagio (Coarse mesh)	0.66	0.46	22	0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

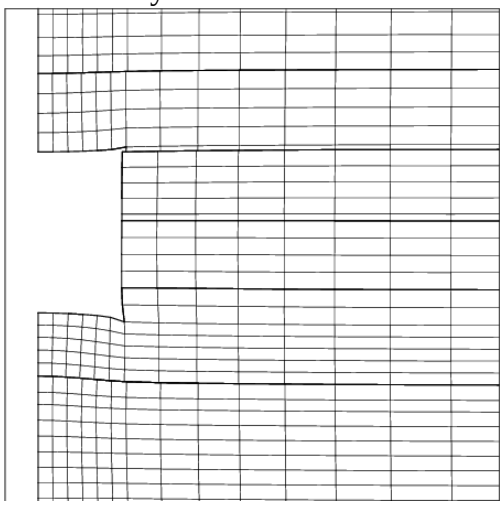
Predicted deformed shapes of Room B using both a coarse mesh (consisting of 5032 nodes and 2184 elements and is one element thick in the out of plane direction with $\Delta Z_{\text{element}}$ = 0.45 m) and the reference mesh, shown previously in Figure 4-12 (containing 28284 nodes and 13248 elements), 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.

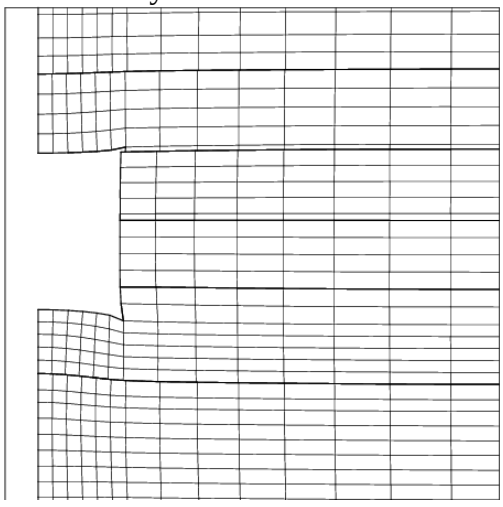


Time = 0.0 year


Time = 1.0 year


Time = 2.0 years


Time = 3.0 years


Time = 4.0 years

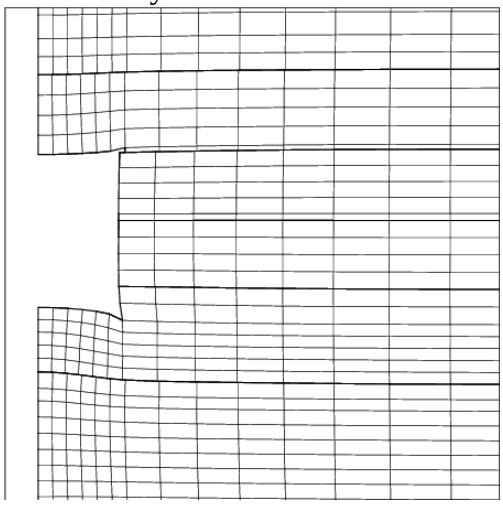
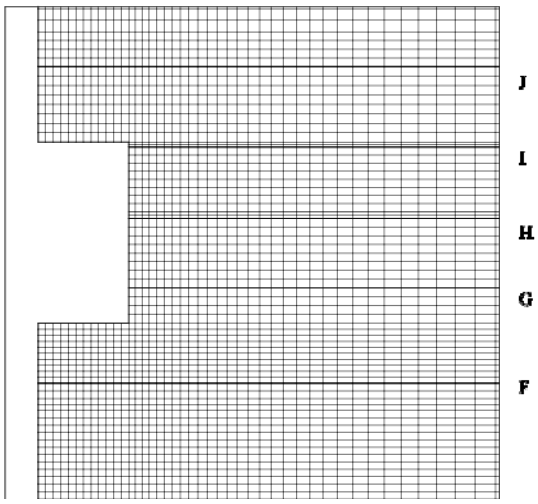
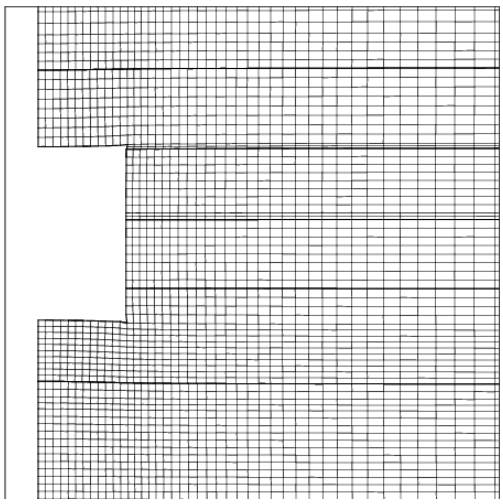

Time = 5.0 years

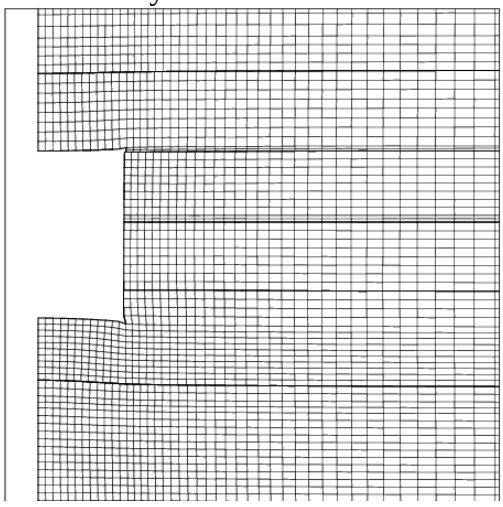
Figure 4-20 Coarse Mesh Structural Simulation: Deformation vs. Time Snapshots



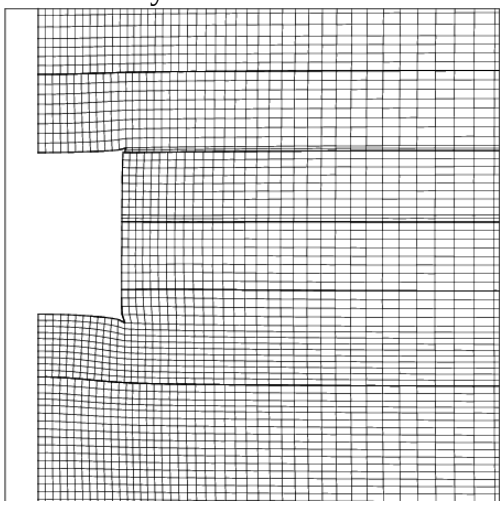
Time = 0.0 year



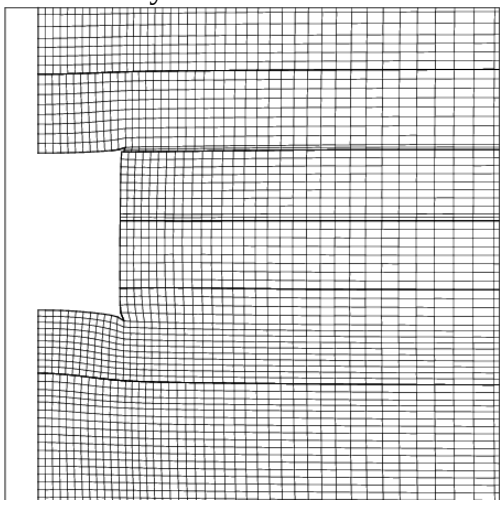
Time = 1.0 year



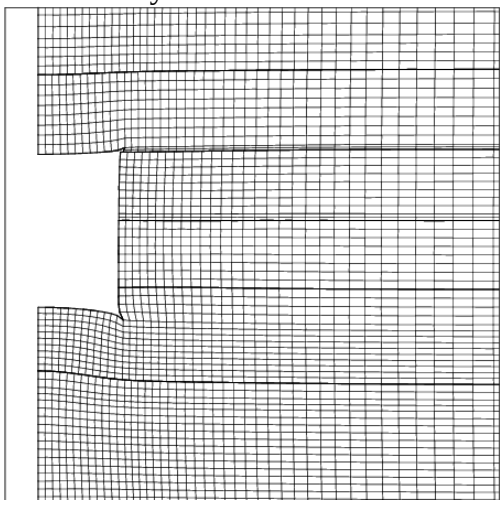
Time = 2.0 years



Time = 3.0 years



Time = 4.0 years



Time = 5.0 years

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.

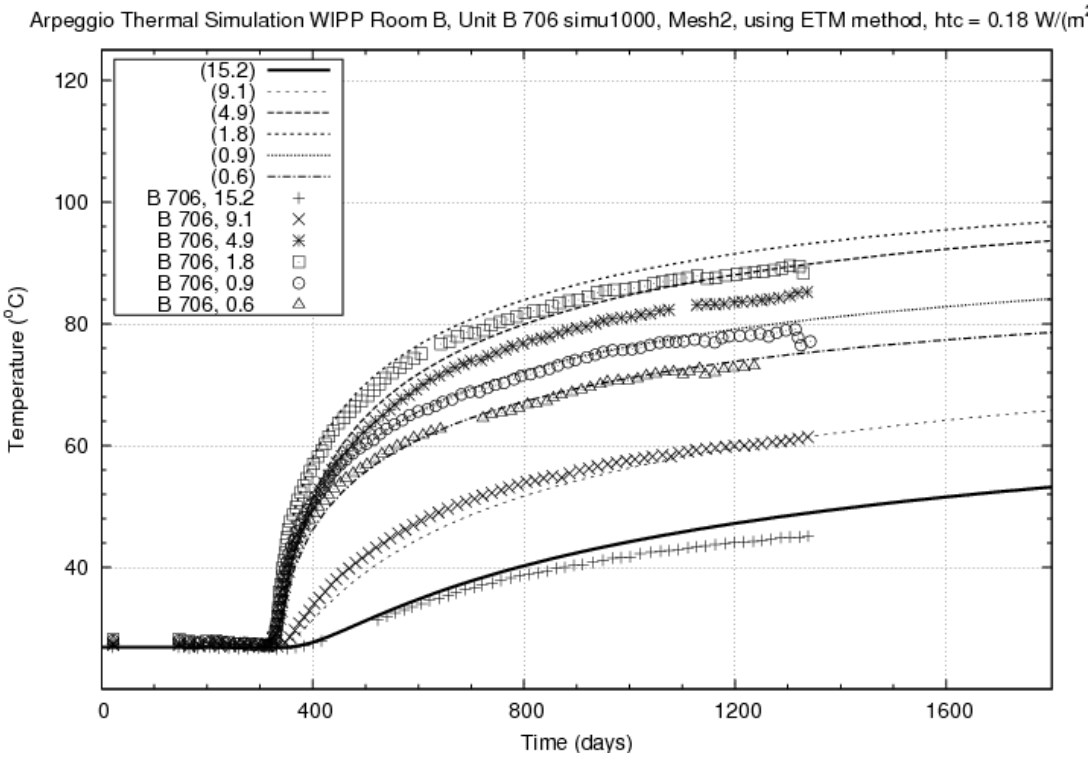


Figure 5-1 Heated Room Coupled Calculation, Using Equivalent Thermal Material, Response Compared To Measured Thermocouple B-706 Temperatures

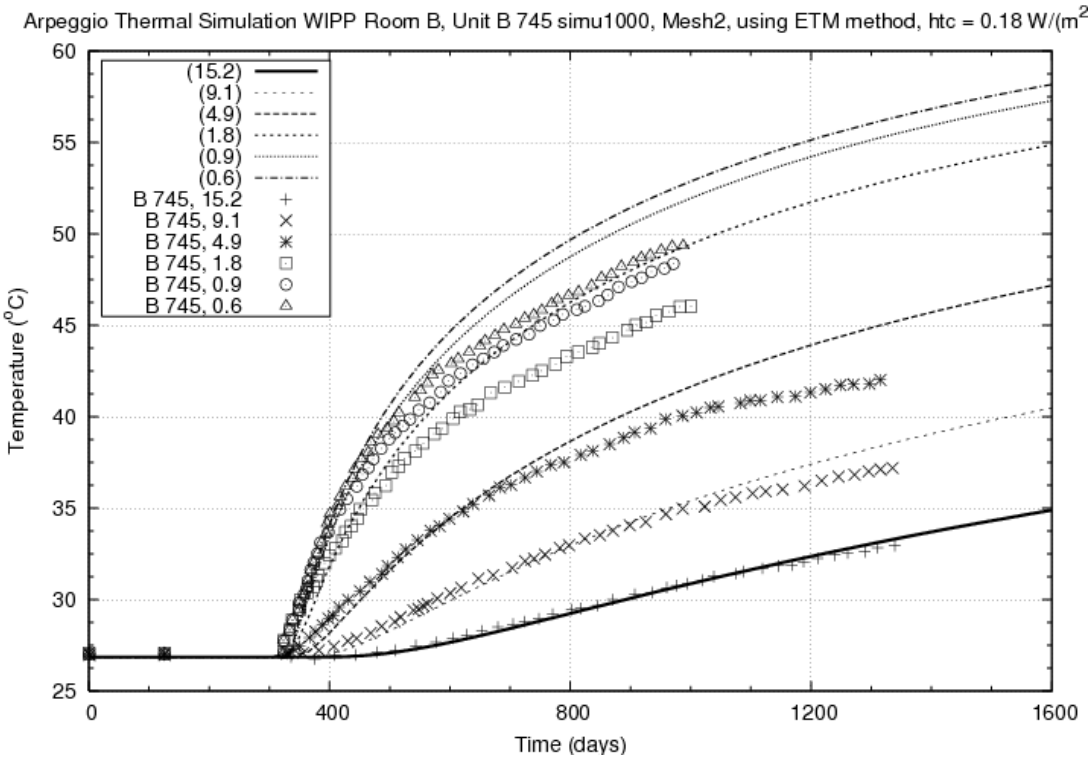


Figure 5-2 Heated Room Coupled Calculation, Using Equivalent Thermal Material, Response Compared To Measured Thermocouple B-745 Temperatures

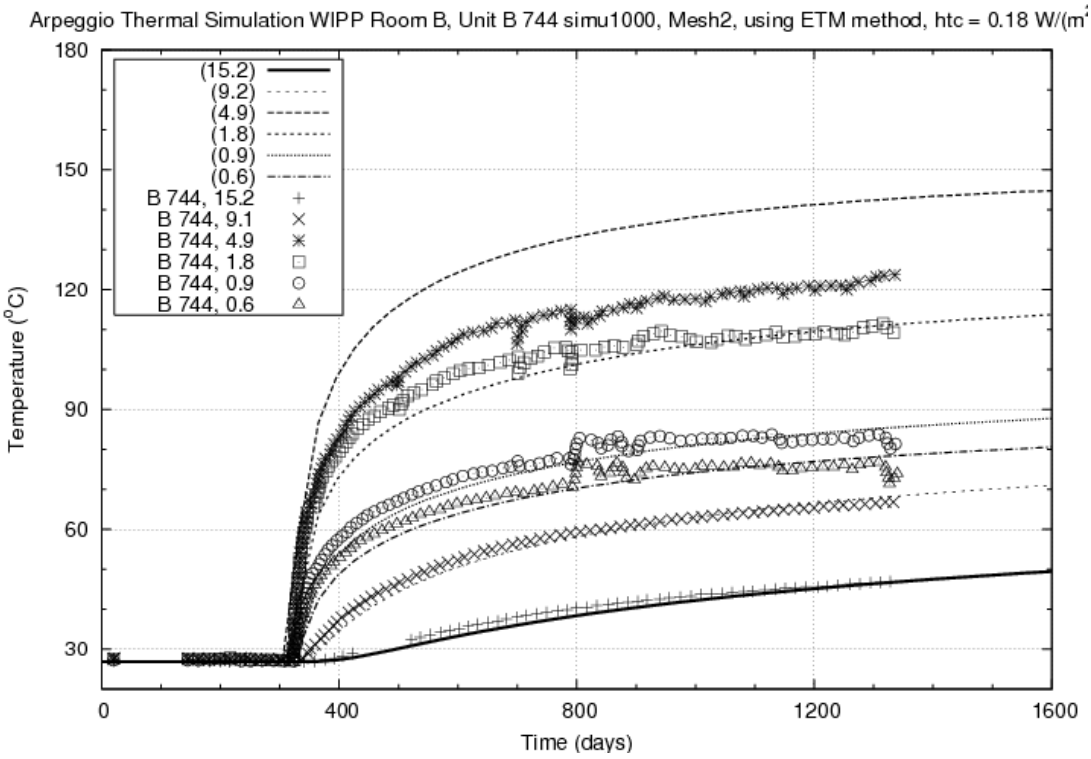


Figure 5-3 Heated Room Coupled Calculation, Using Equivalent Thermal Material, Response Compared To Measured Thermocouple B-744 Temperatures

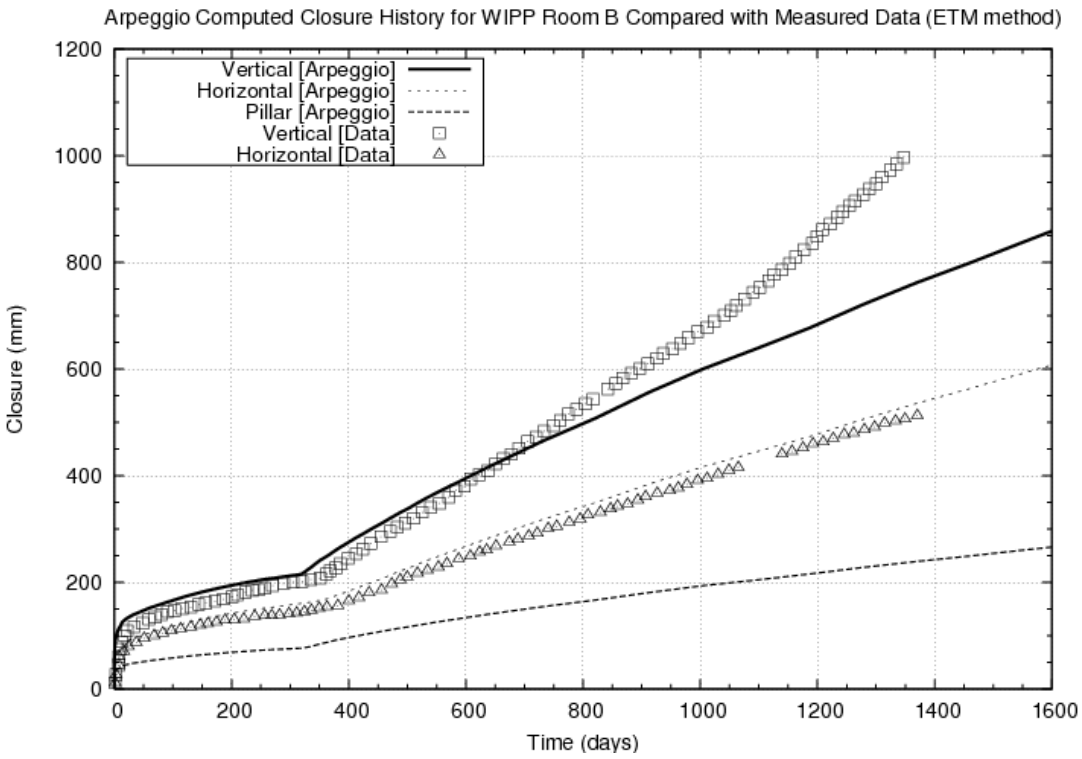


Figure 5-4 Heated Room Coupled Calculation, Using Equivalent Thermal Material, Response Compared To Measured Extensometer Data

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

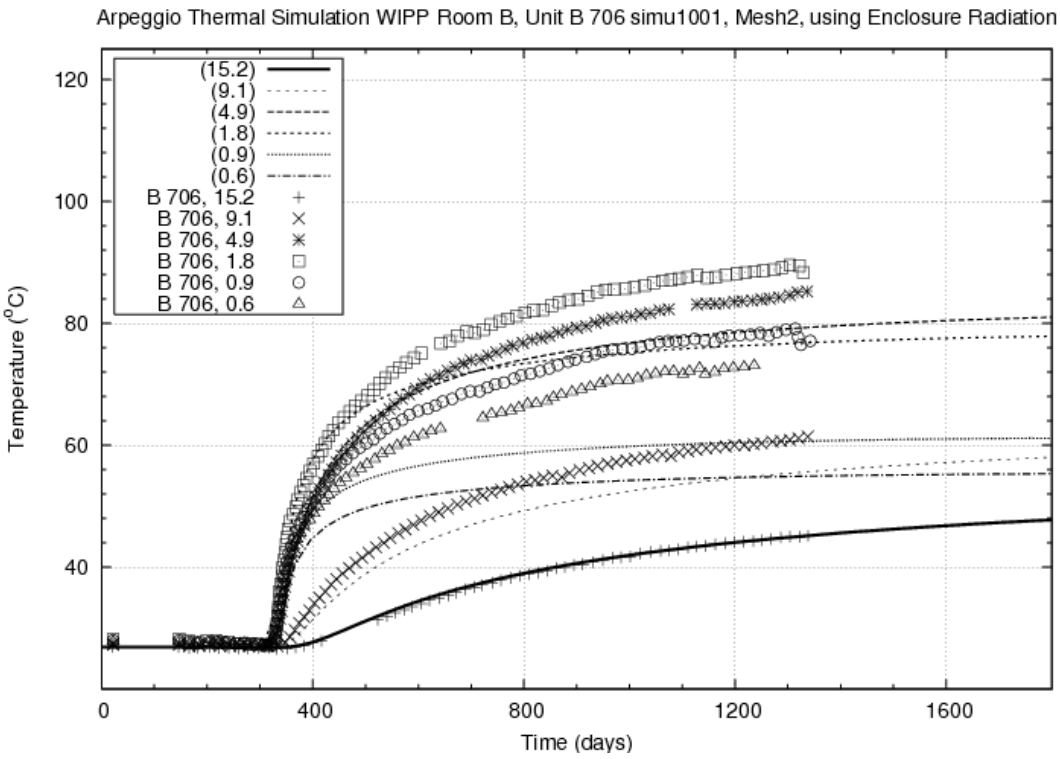


Figure 5-6 Heated Room Coupled Calculation, Using Enclosure Radiation, Response Compared To Measured Thermocouple B-706 Temperatures

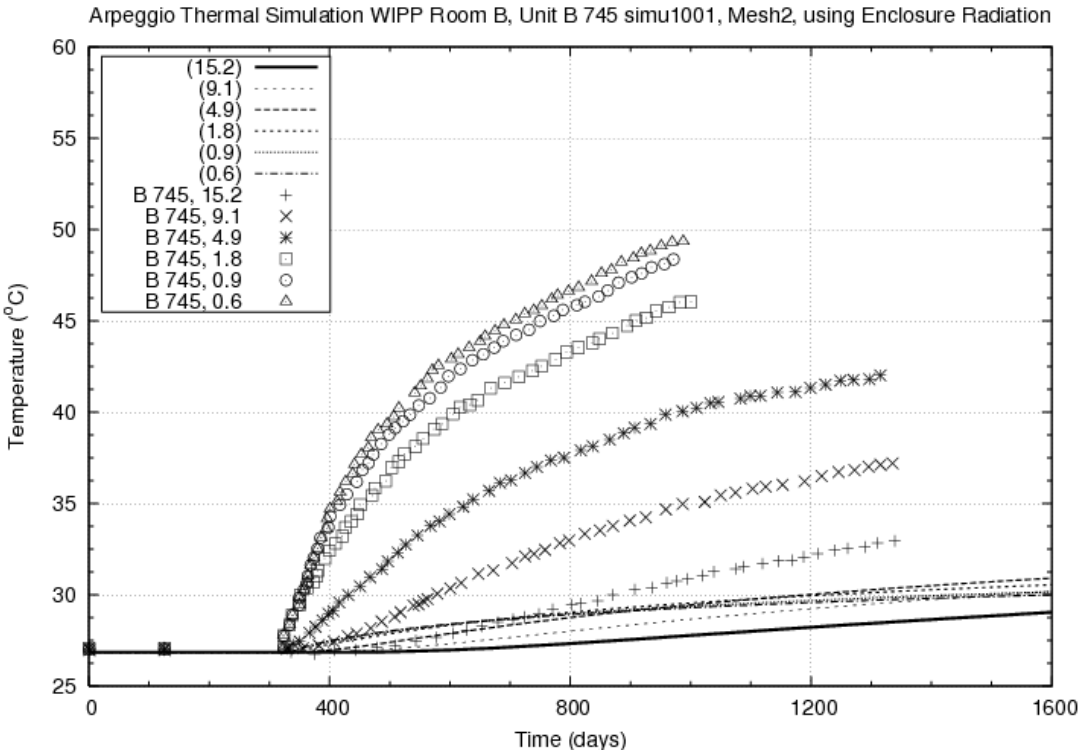


Figure 5-7 Heated Room Coupled Calculation, Using Enclosure Radiation, Response Compared To Measured Thermocouple B-745 Temperatures

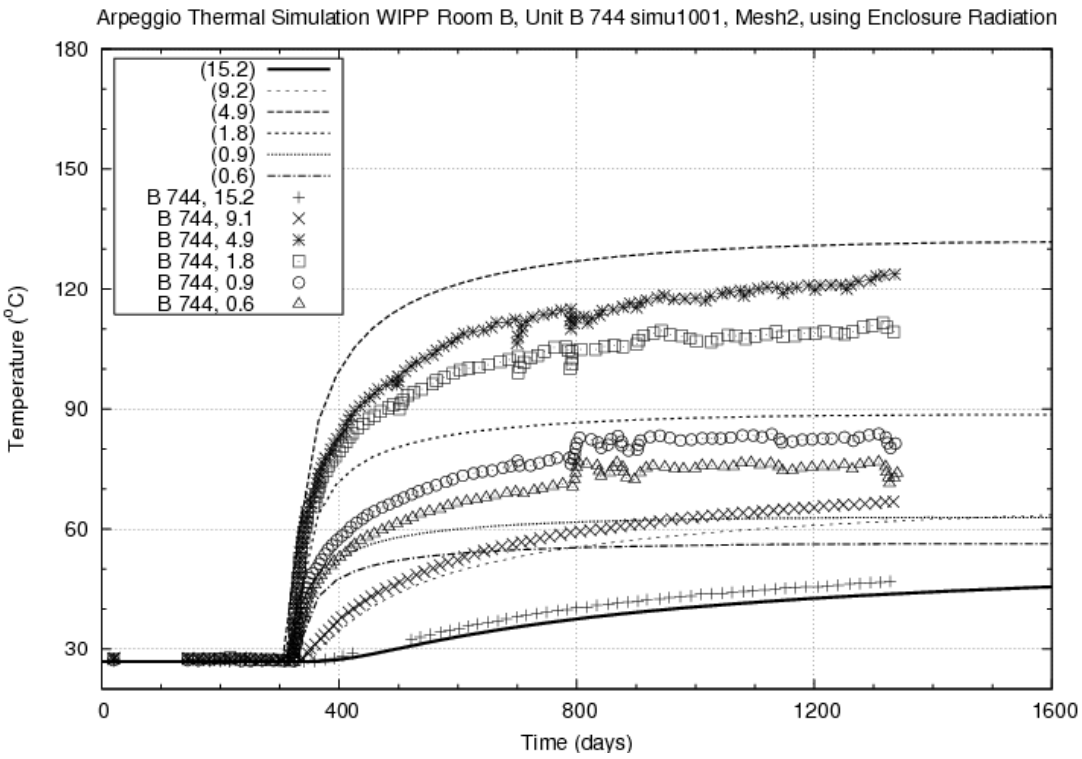


Figure 5-8 Heated Room Coupled Calculation, Using Enclosure Radiation, Response Compared To Measured Thermocouple B-744 Temperatures

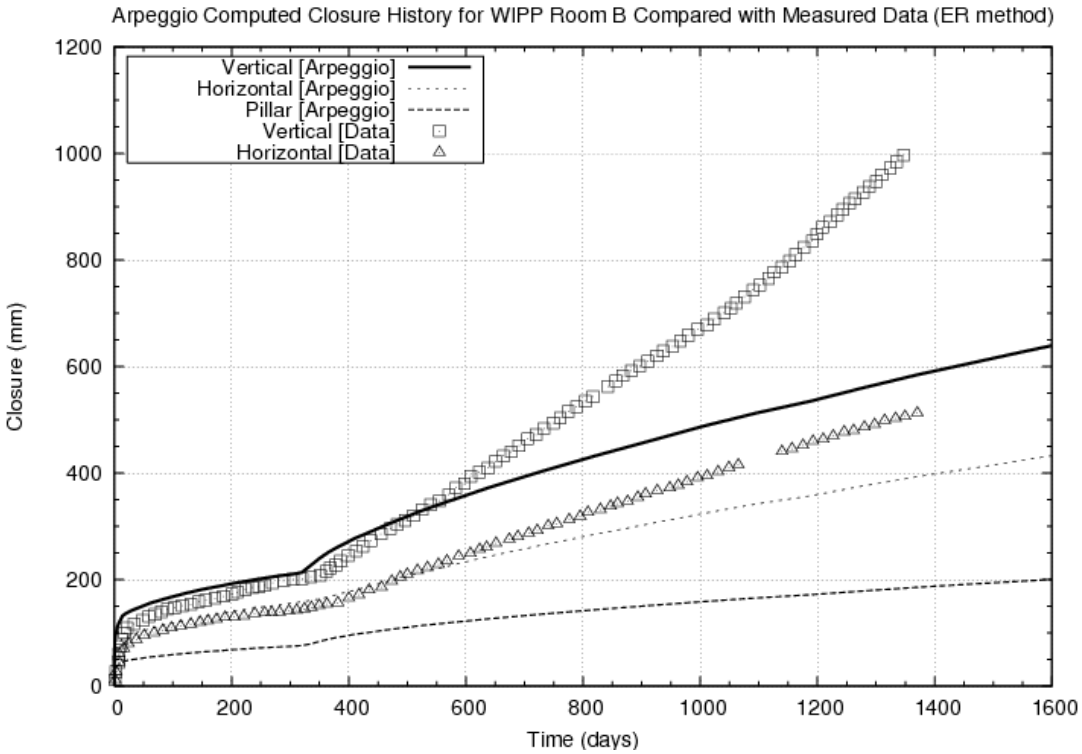


Figure 5-9 Coupled Calculation Heated Room Closure, Using Enclosure Radiation, Response Compared To Measured Extensometer Data

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 ºC (9 ºF) 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 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.

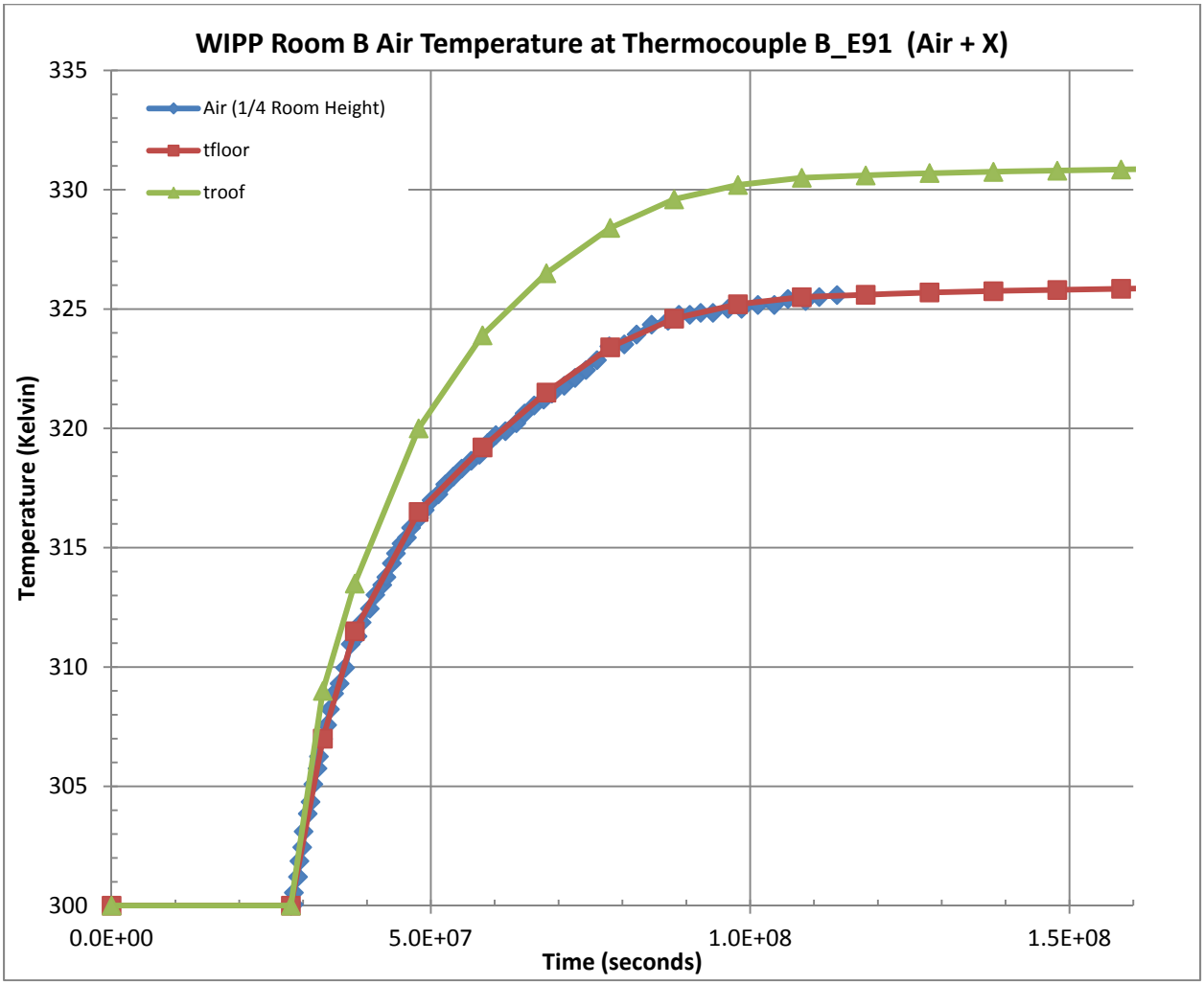


Figure 5-10 Dirichlet Temperature Boundary Condition Model and Measured Thermocouple B-E91 Temperature (model=red and green; data=blue)

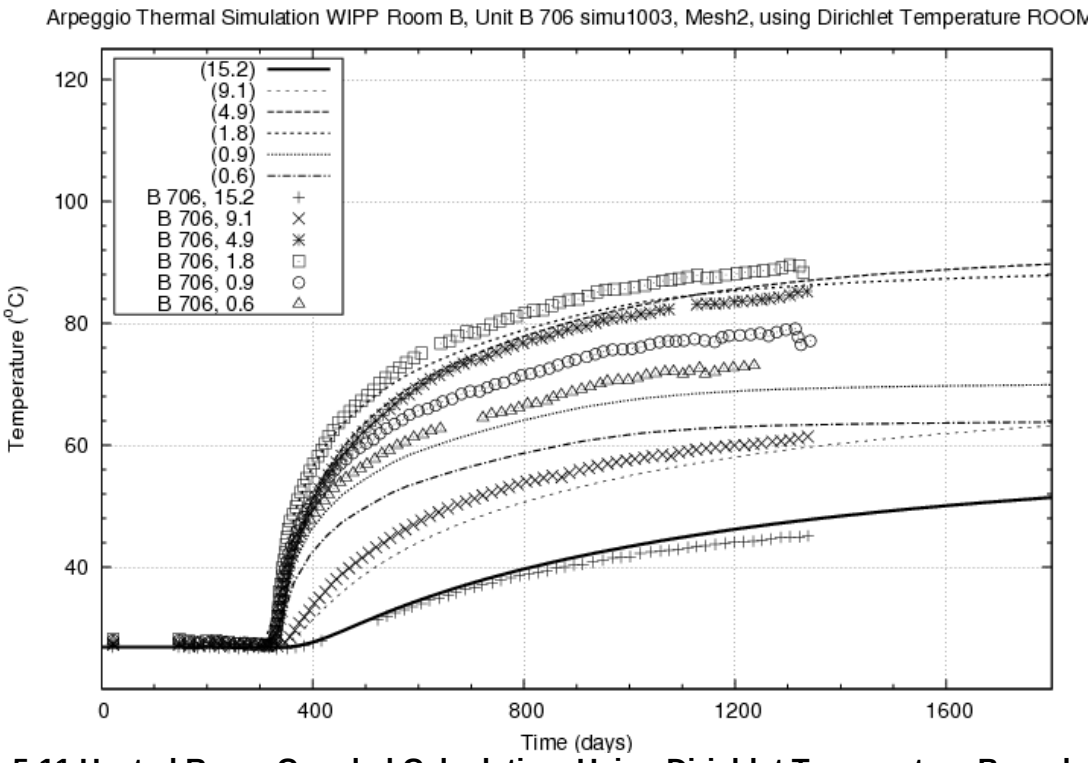


Figure 5-11 Heated Room Coupled Calculation, Using Dirichlet Temperature Boundary Condition, Response Compared To Measured Thermocouple B-706 Temperatures

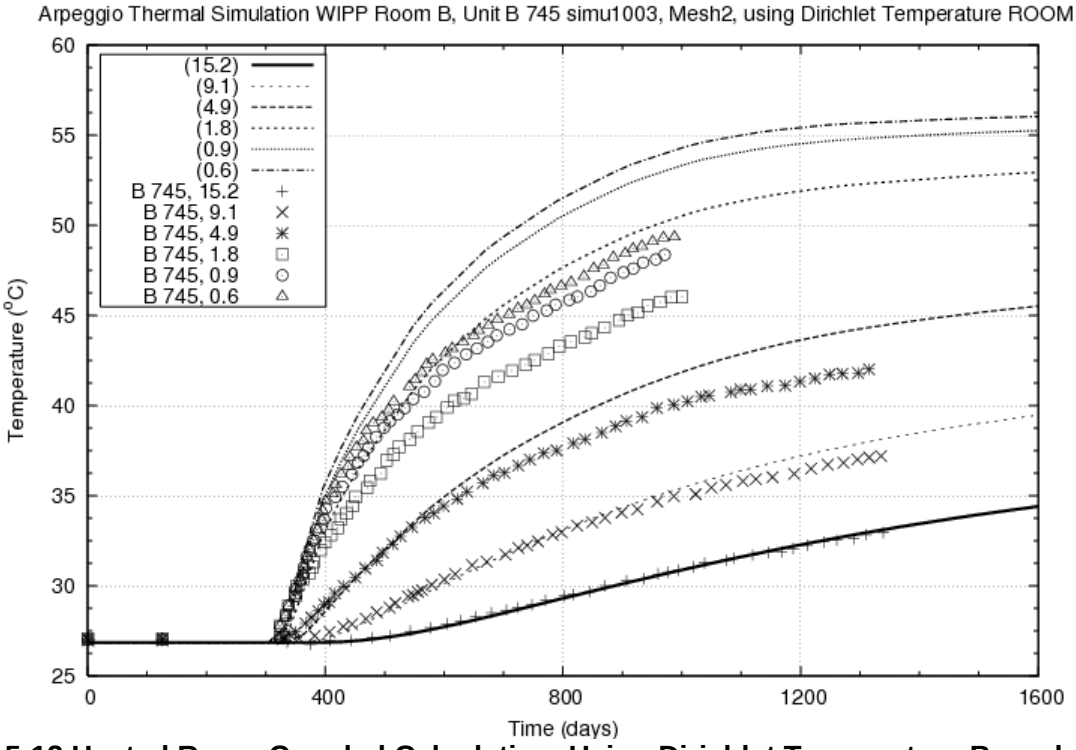


Figure 5-12 Heated Room Coupled Calculation, Using Dirichlet Temperature Boundary Condition, Response Compared To Measured Thermocouple B-745 Temperatures

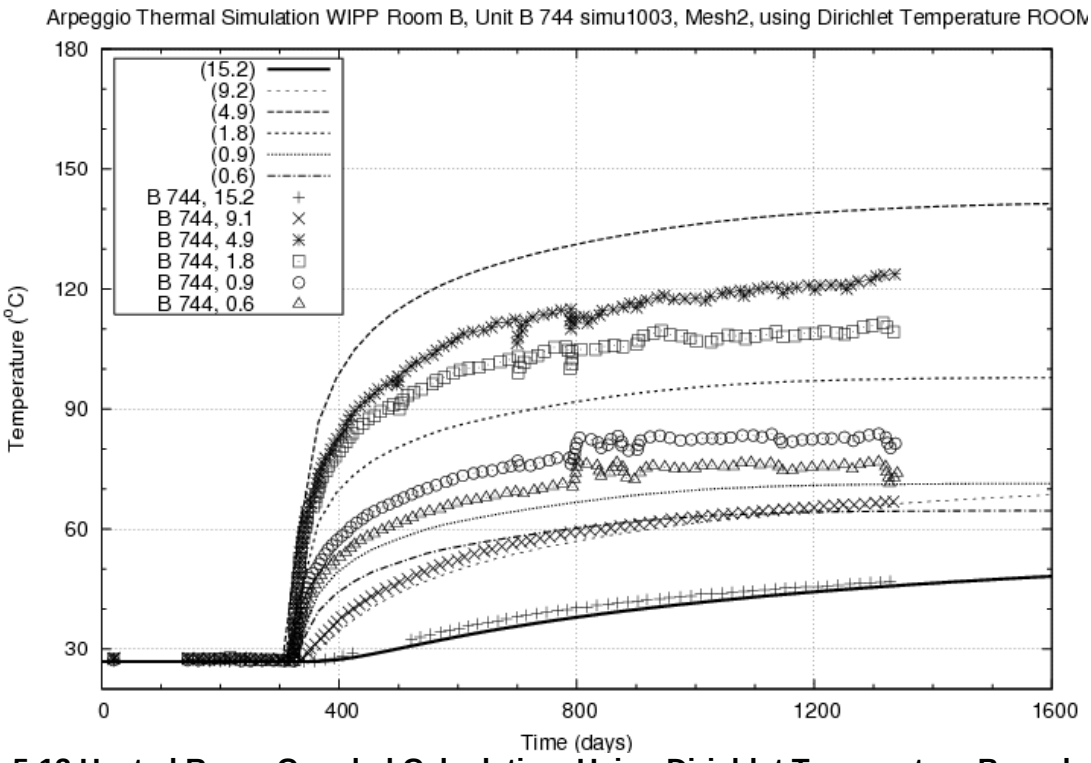


Figure 5-13 Heated Room Coupled Calculation, Using Dirichlet Temperature Boundary Condition, Response Compared To Measured Thermocouple B-744 Temperatures

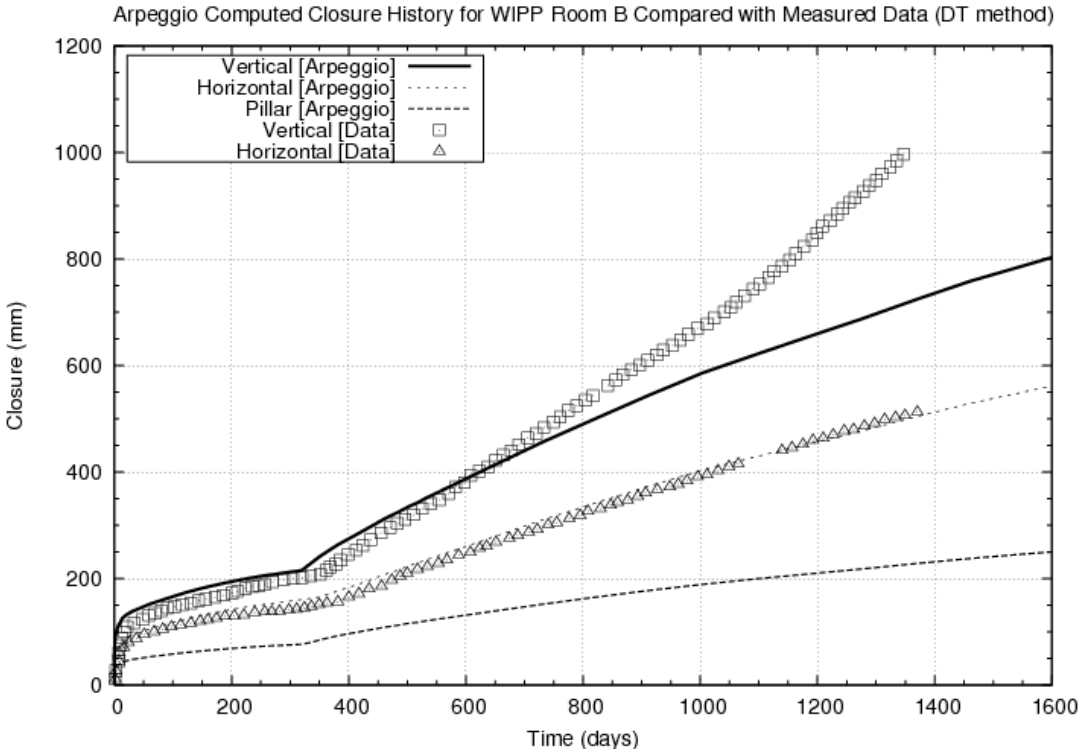


Figure 5-14 Coupled Calculation Heated Room Closure, Using Dirichlet Temperature Boundary, Response Compared To Measured Extensometer Data

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.

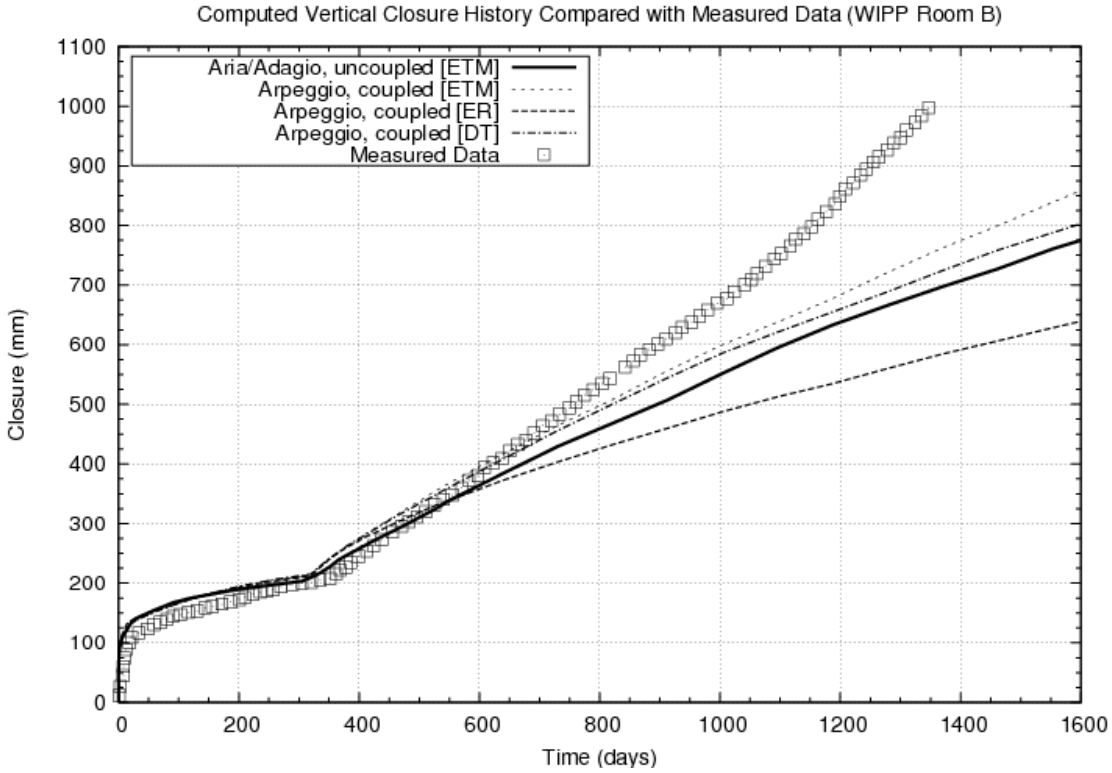


Figure 5-15 Numerical Predictions Of Heated Room Vertical Closure Compared To Measured Extensometer Data

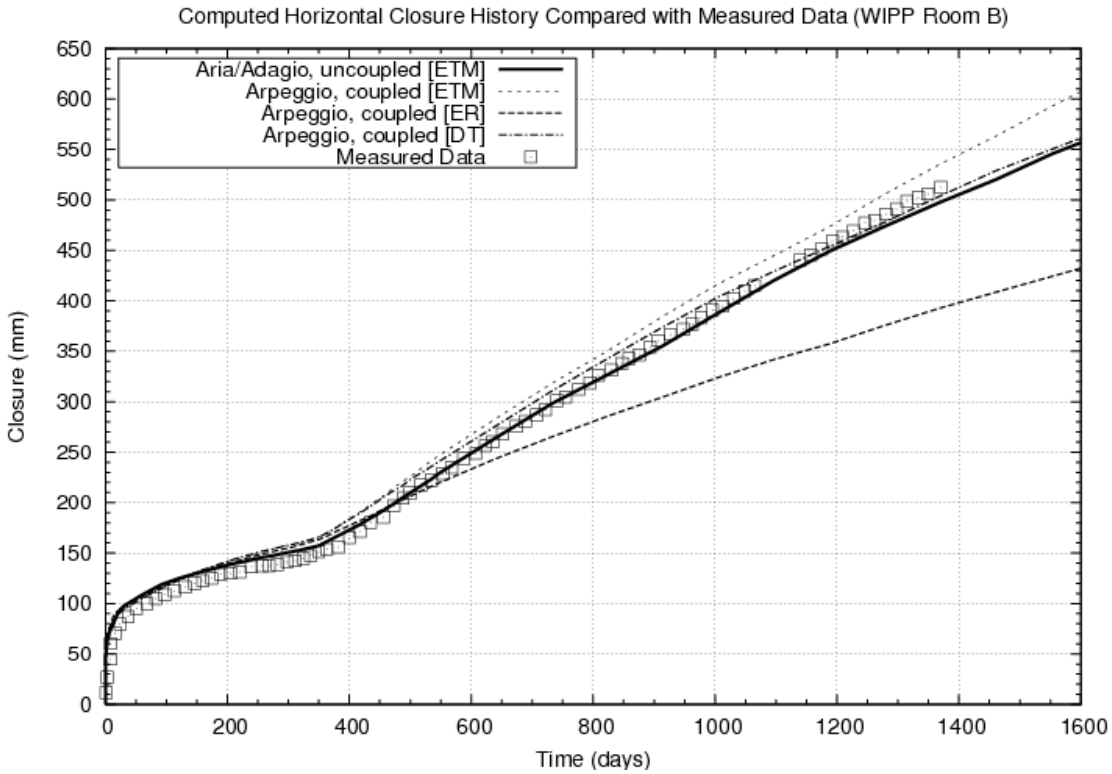


Figure 5-16 Numerical Predictions of Heated Room Horizontal Closure Compared To Measured Extensometer Data

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-

287), 2010). 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

A constitutive model for inelastic flow and damage evolution in solids under triaxial compression. **Chan, K.S., et al. 1992.** s.l. : Mech Mat, 1992, Vol. 14, pp. 1-14.

A model for rock salt, describing transient, stationary, and accelerated creep and dilatancy. **M., Gunther R. and Salzer, K. 2007.** [ed.] K. H. Lux, Wolfgang Minkley, and Jr. H. Reginald Hardy Manfred Wallner. London : Taylor and Francis Group, 2007. The Mechanical Behavior of Salt: Understanding of THMC Processes in Salt; Proceedings of the 6th Conference (SaltMech6), Hannover, Germany, 22-25 May.

Benchmarking of geomechanical constitutive models for rock salt (ARMA-10-287). **Hampel, A., et al. 2010.** Salt Lake City, NV : Proc. American Rock Mechanics Association (ARMA) 44th US Rock Mechanics Symposium, 27-30 June 2010, 2010. ARMA-10-287.

Biffle, J. H. 1993. *JAC3D : a three-dimensional finite element computer program for the nonlinear quasi-static response of solids with the conjugate gradient method.* Albuquerque, NM : Sandia National Laboratories, 1993. SAND87-1303.

Callahan, G. D., Fossum, A. F. and Svalstad, D. K. 1986. *Documentation of SPECTROM-32: a finite element thermomechanical stress analysis program.* Rapid City, SD : RE/SPEC Inc., 1986. RSI-0269.

Chan, K.S., et al. 1996. *A Constitutive Model for Representing Coupled Creep, Fracture, and Healing in Rock Salt.* Albuquerque, NM : Sandia National Laboratories, 1996. SAND96-0376C.

Cubit. 2012. *A Finite Element Method Meshing Tool.* Albuquerque, NM : Sandia National Laboratories, 2012. Version 13.1, Build 47471.

D. E. Munson, R. L. Jones, J. R. Ball, R. M. Clancy, D. L. Hoag, and S. V. Petney. 1990. *Overtest for Simulated Defense High-Level Waste (Room B): In Situ Data Report (May 1984 - February 1988) Waste Isolation Pilot Plant (WIPP) Thermal/Structural Interactions Program.* Albuquerque : Sandia National Laboratories, 1990. SAND89-2671.

Damage-induced nonassociated inelastic flow in rock salt. **Chan, K.S., et al. 1994.** s.l. : International Journal of Plasticity, 1994, Vol. 10 (6), pp. 623-642.

DeVries, K. L., Mellegard, K. D. and Callahan, G.D. 2002. *Salt Damage Criterion Proof-of-Concept Research.* Rapid City, SD : RESPEC, 2002. Topical Report RSI-1675 (DE-FC26-00NT41026).

Fossum, A.F., et al. 1988. *How Should One-Dimensional Laboratory Equations be Cast in Three-Dimensional Form?* Minneapolis, MN : Key Questions in Rock Mechanics: Brookfield: McGraw-Hill Book Company, 1988.

George, O.L. 1984. *Simulation of Radiant Heat Transfer in a WIPP Drift by Use of a Fictitious Conductive Medium," Memorandum to R. D. Krieg, June 9, 1984.* Albuquerque, NM : Sandia National Laboratories, 1984.

Kreig, R.D., Powers, D. and Price, R.H. 1982. Proposed September 1982 WIPP stratigraphy", Memorandum to D. E. Munson September 20, 1982. Albuquerque, NM : Sandia National Laboratories, 1982.

Krieg, R.D. 1984. *Reference Stratigraphy and Rock Properties for the Waste Isolation Pilot Plant (WIPP) Project.* Albuquerque, NM : Sandia National Laboratories, 1984. SAND83-1908.

Matalucci, R. V., Christensen, C. L., Hunter, T. O., Molecke, M. A., & Munson, D. E. 1982. *Waste Isolation Pilot Plant (WIPP) Research and Development Program: In Situ Testing Plan, March 1982.* Albuquerque : Sandia National Laboratories, 1982. SAND81-2628.

Matalucci, R.V, et al. 1982. *Waste Isolation Pilot Plant (WIPP) Research and Development Program: In Situ Testing Plan, March 1982.* Albuquerque, NM : Sandia National Laboratories, 1982. SAND81-2628.

Miller, J.D. 1981. *Computations in Support of the Design Verification Long Constant Cross-Section Room, Memorandum to R. V. Matalucci Novermber 23, 1981.* Albuquerque, NM : Sandia National Laoratories, 1981.

Morgan, H. S. and Stone, C. M. 1985. *Pretest Reference Calculation for the Overtest for Simulated Defense High Level Waste (WIPP Room B In Situ Experiment).* Albuquerque, NM : Sandia National Laboratories, 1985. SAND85-0213.

Morgan, H.S, Krieg, R.D. and Matalucci, R.V. 1981. *Comparative Analysis of Nine Structural Codes Used in the Second WIPP Benchmark Problem.* Albuquerque, NM : Sandia National Laboratories, 1981. SAND81-1389.

Munson, D.E. 2002. *Analysis (micromechanical origin) of Reversible Creep Strains in Rocksalt - A Two State Variable M-D Creep Model.* Albuquerque, NM : Sandia National Laboratories, 2002. SAND2002-0355C.

Munson, D.E. and Dawson, P. R. 1979. *Constitutive Model for the Low Temperature Creep of Salt (With Application to WIPP).* Albuquerque, NM : Sandia National Laboratories, 1979. SAND79-1853.

—. 1982. *A Transient Creep Model for Salt during Stress Loading and Unloading.* Albuquerque, NM : Sandia National Laboratories, 1982. SAND82-0962.

Munson, D.E. 1997. *Constitutive Model of Creep in Rock Salt Applied to Underground Room Closure.* s.l. : International Journal of Rock Mechanics, Mineralogy and Science, Elsevier Science Ltd., Volume 34, No. 2, pp. 233-247., 1997.

—. 1979. *Preliminary Deformation-Mechanism Map for Salt (with Application to WIPP).* Albuquerque, NM : Sandia National Laboratories, 1979. SAND79-0076.

Munson, D.E., DeVries, K.L. and Callahan, G.D. 1990. *Comparison of Calculations and In Situ Results For a Large, Heated Test Room at the Waste Isolation Pilot Plant (WIPP).* Albuquerque, NM : Sandia National Laboratories, 1990. SAND89-2268.

Munson, D.E., et al. 1988. *Mining Development Test (Room D): In Situ Data Report (March 1984 - May 1988) Waste Isolation Pilot Plant (WIPP) Thermal/Structural Interactions Program.* Albuquerque, NM : Sandia National Laboratories, 1988. SAND88-1460.

Munson, D.E., et al. 1990. *Overtest for Simulated Defense High-Level Waste (Room B): In Situ Data Report (May 1984 - February 1988) Waste Isolation Pilot Plant (WIPP) Thermal/Structural Interactions Program.* Albuquerque, NM : Sandia National Laboratories, 1990. SAND89-2761.

Munson, D.E., Fossum, A.F. and Senseny, P.E. 1989. *Advances in Resolution of Discrepancies between Predicted and Measured in Situ WIPP Room Closures.* Albuquerque, NM : Sandia National Laboratories, 1989. SAND88-2948.

—. 1989. *Advances in Resolution of Discrepancies between Predicted and Measured in Situ WIPP Room Closures.* Albuquerque, NM : Sandia National Laboratories, 1989. SAND88-2948.

Notz, P.K., et al. 2007. *Aria 1.5: User Manual.* Albuquerque, NM : Sandia National Laboratories, 2007. SAND2007-2734. SAND2007-2734.

Salt Constitutive Modeling using Mechanism Maps. **Munson, D.E. and Dawson, P. R. 1984.** s.l. : Clausthal-Zellerfeld: Trans Tech Publications, 1984. Proc. 1st International Conference on the Mechanical Behavior of Salt.

SIERRA Mechanics for Coupled Multi-Physics Modeling of Salt Repositories. **Arguello, J.A. and Rath, J.S. 2011.** Albuquerque, NM : CRC Press/Balkema, 2011. SaltMech7 - 7th International Conference on the Mechanical Behavior of Salt.

SIERRA: A Software Environment for Developing Complex Multi-Physics Applications. **Edwards, H. C., & Stewart, J. R. 2001.** Amsterdam : Elsevier, 2001. In K. J. Bathe (ed.), First MIT Conference on Computational Fluid and Solid Mechanics.

Stone, C. M. 1983. *Analyses of the Heated WIPP In-Situ Experiments," Memorandum to D. E. Munson, February 16, 1983.* Albuquerque, NM : Sandia National Laboratories, 1983.

—. 1990. *SANTOS – a two-dimensional finite element program for the quasistatic, large deformation, inelastic response of solids.* Albuquerque, NM : Sandia National Laboratories, 1990. SAND84-2618.

Stone, C.M., Krieg, R.D. and Beisinger, Z.E. 1985. *SANCHO - A Finite Element Computer Program for the Quasistatic, Large Deformation, Inelastic Response of Two-Dimensional Solids.* Albuquerque, NM : Sandia National Laboratories, 1985. SAND85-2618.

Stone, C.M., Krieg, R.D. and Branstetter, L.J. 1981. *The Effects of Clay Seam Behavior on WIPP Repository Design.* Albuquerque, NM : Sandia National Laboratories, 1981. SAND81-0768.

Svalstad, D.K. 1989. *Documentation of SPECTROM-41: A finite element heat transfer analysis program.* Albuquerque, NM : Sandia National Laboratories, 1989. SAND88-7122 (contractor report).

Team, SIERRA Solid Mechanics. 2010. *Adagio 4.18 User's Guide.* Albuquerque : Sandia National Laboratories, 2010. SAND2010-6313.

The composite dilatancy model: A constitutive model for the mechanical behavior of rock salt. **A., Hampel. 2007.** [ed.] K. H. Lux, Wolfgang Minkley, and Jr. H. Reginald Hardy Manfred Wallner. London : Taylor and Francis Group, 2007. Proceedings of the 6th Conference (SaltMech6), Hannover, Germany, 22-25 May.

Wang, Y., et al. 2011. *Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Integrated Performance and Safety Codes (IPSC): gap Analysis for High Fidelity and Performance Assessment Code Development.* Albuquerque : Sandia National Laboratories, 2011. SAND2011-1831.

Wellman, G.W. 1999. *MAPVAR - A Computer Program to Transfer Solution Data Between Finite Element Meshes.* Albuquerque, NM : Sandia National Laboratories, 1999. SAND99-0466.

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

    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 = nodelist_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

end 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 vonmis
  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)                      #
#                              = Pascal                              #
#                 energy       = Newton*m                            #
#                              = Joule                               #
#                 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 <= 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 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
      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
```

```
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
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


    End Aria Region AriaRegion

  End procedure AriaProcedure

END SIERRA roomb_thermal
```

```
#-------------------------------------------------------------------#
#     directory : /home/jsrath/projects/NEAMS/roomb/structural/simu106
#          file : adagio.i                                          #
#        author : Jonathan Scott Rath                               #
#   description : NEAMS WIPP Room B Adagio input deck               #
#                 Model 1 (Room B, Structural)                      #
#  revision_log : 01/SEPTEMBER/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)                     #
#                              = Pascal                             #
#                 energy       = Newton*m                           #
#                              = Joule                              #
#                 power        = Joule/sec                          #
#                              = Newton*m/sec                       #
#                              = Watt                               #
#-------------------------------------------------------------------#

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  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)
                     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 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 anhydrite

  Begin 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/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

###
### 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
      End History Output adagio_history

###
### 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:       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

###
### 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

J. Guadalupe Argüello and Jonathan S. Rath
Computational Structural Mechanics & Applications Department, Sandia National Laboratories, Albuquerque, NM 87185-0372, USA

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. An effort on high-fidelity continuum modeling was undertaken to exercise the existing SIERRA Mechanics code suite. A series of simulations and their results will be presented and discussed herein to illustrate some of the capabilities available in SIERRA Mechanics for simulating salt repositories.

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.

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

application to another; a solution controller for code coupling; and 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-Hydrological-Mechanical-Chemical (THMC) coupling, with adaptive solution control, in a repository-setting are Aria (Notz et al. 2007) and Adagio (SIERRA Solid Mechanics 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 mechanics portion of the THMC coupling is handled by Adagio. It solves for the quasi-static, large deformation, large strain behavior of nonlinear solids in three dimensions. Adagio has some discriminating Sandia-developed technology for solving solid mechanics problems that involves matrix-free iterative solution algorithms for efficient solution of extremely large and highly nonlinear problems. This technology is well-suited for scalable implementation on massively parallel computers. The THMC coupling is done through a solution controller within SIERRA Mechanics called Arpeggio.

In this work we describe the application of the SIERRA Mechanics code suite to a set of salt repository problems recently exercised to validate its applicability to this class of problems and to demonstrate its use on anticipated more-complex coupled simulations of future nuclear waste salt repositories. We describe its use on the following problems of interest: the simulation of the isothermal WIPP Mining Development Test (Room D) Thermal/Structural Interactions in-situ experiment (Munson et al. 1988); the simulation of the WIPP Overtest for Simulated Defense High-Level Waste (Room B) Thermal/Structural Interactions in-situ experiment (Munson et al. 1990b); and another recent simulation of a generic salt repository for high-level waste (Stone et al. 2010). Results from the various simulations will be presented and discussed to illustrate the capabilities available in SIERRA Mechanics for simulating salt repositories.

2 DESCRIPTION OF AND RESULTS FOR WIPP CONFIGURATIONS

Several large-scale in-situ tests were fielded underground at the Waste Isolation Pilot Plant (WIPP) during an 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 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 toolset, will first 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. (1989) 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.

$$\dot{\varepsilon}_s = \sum_{i=1}^{3} \dot{\varepsilon}_{s_i} \tag{1}$$

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.

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

$$\dot{\varepsilon}_{ss_2} = A_2 \left(\frac{\sigma_{eq}}{G} \right)^{n_2} e^{\frac{-Q_2}{RT}} \tag{3}$$

$$\dot{\varepsilon}_{ss_3} = \left(B_1 e^{-Q_1/RT} + B_2 e^{-Q_2/RT} \right) \sinh\left[q \left(\frac{\sigma_{eq} - \sigma_0}{G} \right) \right] \times H\left(\sigma_{eq} - \sigma_0\right) \tag{4}$$

where σ_{eq} is the equivalent stress; T is the temperature (absolute); G is the shear modulus; A_1, A_2, B_1, & B_2 are structure factors; Q_1 & Q_2 are activation energies; R is the universal gas constant; q is the activation volume, σ_0 is the stress limit; and H is the Heaviside function with argument $(\sigma_{eq} - \sigma_0)$.

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 σ_0. 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 σ_1 and σ_3 respectively $(\sigma_1 \geq \sigma_2 \geq \sigma_3)$. Alternatively, the Tresca stress may be written as a function of the Lode angle, ψ, and the second invariant, J_2, of the deviatoric stress tensor, s (with components s_{ij}).

$$\sigma_{eq} = \sigma_1 - \sigma_3 = 2\cos\psi\sqrt{J_2} \tag{5}$$

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

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

$$J_2 = \frac{1}{2} s_{ij} s_{ji} \tag{7}$$

$$J_3 = \frac{1}{3} s_{ij} s_{jk} s_{ki} \tag{8}$$

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 $\dot{\varepsilon}_s$ is the steady state dislocation creep strain rate defined by Equation 1.

$$\dot{\varepsilon}_{eq} = F \dot{\varepsilon}_s \tag{9}$$

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

$$F = \begin{cases} \exp\left[\Delta \left(1 - \frac{\zeta}{\varepsilon_t^f} \right)^2 \right] & \zeta < \varepsilon_t^f \text{ Transient Branch} \\ 1 & \zeta = \varepsilon_t^f \text{ Equilibrium Branch} \\ \exp\left[-\delta \left(1 - \frac{\zeta}{\varepsilon_t^f} \right)^2 \right] & \zeta > \varepsilon_t^f \text{ Recovery Branch} \end{cases} \tag{10}$$

The choice of the particular branch depends on the transient strain limit ε_t^f and the internal variable ζ. 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.

$$\varepsilon_t^f = K_0 e^{cT} \left(\frac{\sigma_{eq}}{G} \right)^m \tag{11}$$

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

$$\dot{\zeta} = \left(F - 1\right)\dot{\varepsilon}_s \tag{12}$$

Δ and δ, appearing in Equation 10, are the work hardening and recovery parameters and are given by Equations 13 and 14 respectively. In these equations α, β, α_r, and β_r are material parameters. Typically the recovery parameter, δ, is taken to be constant (i.e. $\delta = \alpha_r$).

$$\Delta = \alpha + \beta \log\left(\frac{\sigma_{eq}}{G} \right) \tag{13}$$

$$\delta = \alpha_r + \beta_r \log\left(\frac{\sigma_{eq}}{G} \right) \tag{14}$$

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 5.5 m wide by 5.5 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 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, 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, μ=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 symmetry 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 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 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 13.57 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 9.79 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 SIERRA Mechanics calculation is not shown. However, it contains 2184 hexahedral elements and 5032 nodes.

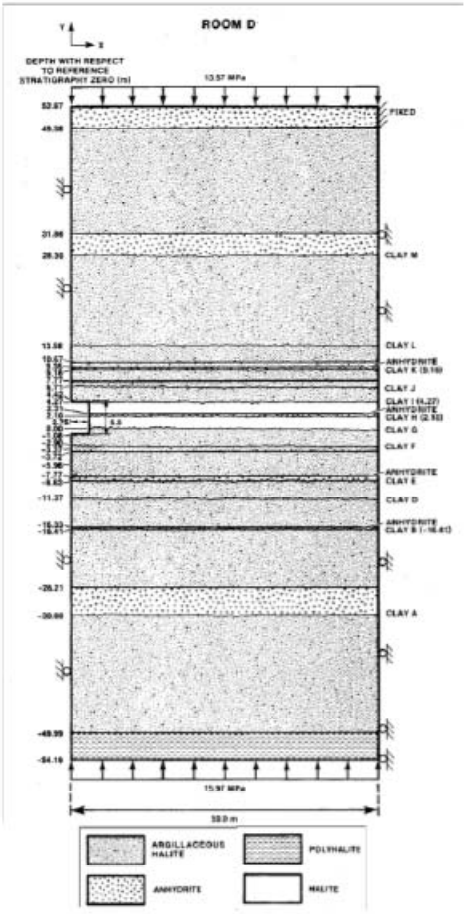


Figure 1. Local stratigraphy around and model of Room D.

2.2.3 *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 1. These parameter are identical to those given in Munson et al. 1989, in an effort to duplicate, as closely as possible, the historical calculation using SIERRA Mechanics in place of the earlier 2D SPECTROM-32 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.

	Parameters		Units	Halite
Elastic Properties	Shear modulus	G	MPa	12,400
	Young's modulus	E	MPa	31,000
	Poisson's ratio	ν	–	0.25
Salt Creep Properties	Structure Factors	A_1	s^{-1}	8.386×10^{22} (1.407×10^{23})
		B_1	s^{-1}	6.086×10^{6} (8.998×10^{6})
		A_2	s^{-1}	9.672×10^{12} (1.314×10^{13})
		B_2	s^{-1}	3.034×10^{-2} (4.289×10^{-2})
	Activation energies	Q_1	cal/mol	25,000
		Q_2	cal/mol	10,000
	Universal gas constant	R	cal/mol -K	1.987
	Absolute temperature	T	K	300
	Stress exponents	n_1	–	5.5
		n_2	–	5.0
	Stress limit of the dislocation slip mechanism	σ_0	MPa	20.57
	Stress constant	q	–	5,335
	Transient strain limit constants	M	–	3.0
		K_0	–	6.275×10^{5} (2.470×10^{6})
		c	K^{-1}	9.198×10^{-3}
	Constants for work-hardening parameter	α	–	-17.37 (-14.96)
		β	–	-7.738
	Recovery parameter	δ	–	0.58

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 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. 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 argillaceous 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. (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.

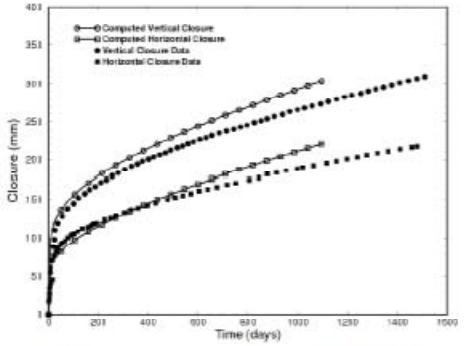


Figure 2. Comparison of calculated (SIERRA Mechanics) and measured in-situ Room D closures.

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. 1990b) 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 2.59 m long (i.e., length of heated cylinder) 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. These 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. (1990a) 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 (Argüello 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 324 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 456 W/m^2 condition on the symmetry plane, only half of this load or 228 W/m^2 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:

$$q = 228\exp\left(-7.327\times10^{-10}t\right) \tag{15}$$

where q is the thermal load in W/m^2 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 Argüello et al., in prep. for additional details). Heat transfer through the salt was modeled with a nonlinear thermal conductivity of the form:

$$\lambda = \lambda_{300}\left(300/T\right)^{\gamma} \tag{16}$$

where λ is the thermal conductivity, T is the absolute temperature in Kelvin, and λ_{300} and γ 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. 1981), 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 2. Thermal properties used in Room B thermal simulations using Aria.

Material		Halite	"Equivalent thermal material"
Density, ρ (kg/m^3)		2300	1
Specific heat, c_p (J/kg/K)		860	1000
Coefficient of linear thermal expansion, α (K^{-1})		45×10^{-6}	N/A
Thermal conductivity parameters	λ_{300} (W/m/K)	5	50
	γ	1.14	0

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:

$$q' \bullet n = h(T - 300) \tag{17}$$

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 $W/m^2/K$) 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 subtler 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:

$$\sqrt{J_2'} = c - aI_1 \tag{18}$$

where J_2' is the modified second deviatoric stress invariant (i.e., $J_2' = \sqrt{3J_2}$), c & a are constants, and I_1 is the first stress invariant. Values of c = 1.35 MPa and a = 0.45 were used for the anhydrite and c = 1.42 MPa and a = 0.473 were used for the polyhalite in the Room B calculation. In addition, the value of the MD Model parameter, K_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 $K_0 = 1.783\times10^6$ is used for the Room B argillaceous halite material.

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 (Argüello 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 probed 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.

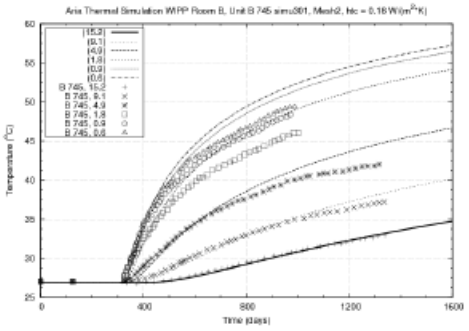


Figure 3. Comparisons of measured in-situ Room B temperatures from thermocouple unit B_745 with computed results from SIERRA Mechanics.

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 probed by the B_706 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 14%, 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 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 scoping 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

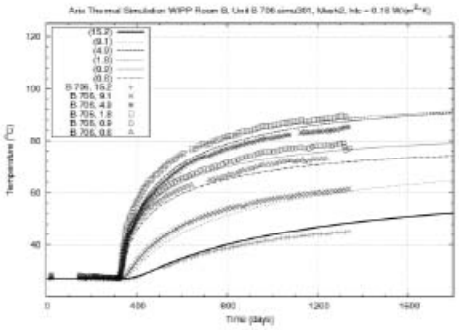


Figure 4. Comparisons of measured in-situ Room B temperatures from thermocouple unit B_706 with computed results from SIERRA Mechanics.

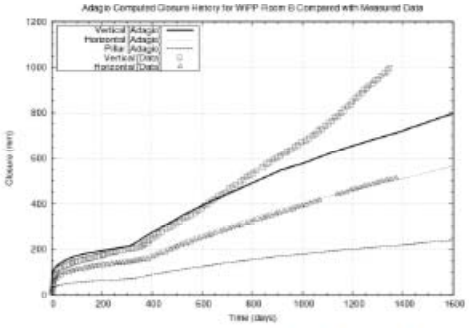


Figure 5. Comparison of measured in-situ Room B closures with computed results from SIERRA Mechanics.

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 tempera-

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 three-dimensional 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 (Bechtold et al. 2004).

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.

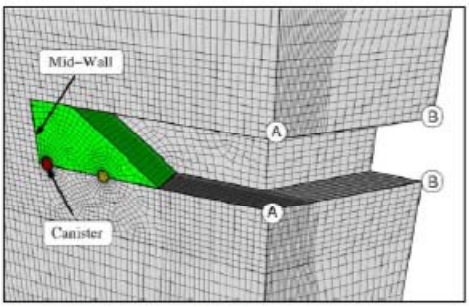


Figure 6. Close-up view of mesh showing the location of points at the alcove and access tunnel corners.

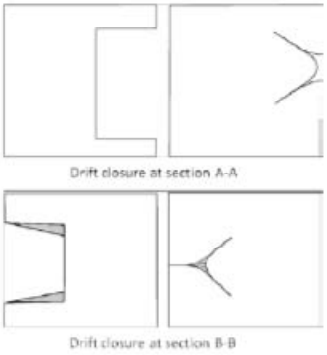


Figure 7. Un-deformed (t=0) and deformed (t=~60 years) views of the access tunnel looking from the back of the model toward the alcove/access-tunnel intersection (upper) and vice-versa (lower).

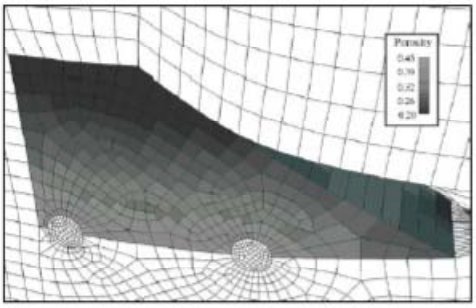


Figure 8. Porosity in the crushed salt backfill at 8 years for the MD model simulation with an initial emplaced porosity of 42%.

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 in-situ 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 the 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

Argüello, J.G., Wang, Y., Freeze, G.A., Davison, S.M., Jove-Colon, C.F., Lee, J.H., Mariner, P., & Rath, J.S. 2011. Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Integrated Performance and Safety Codes (IPSC): Fiscal Year 2011 Challenge Problem Progress Report. SAND2012-XXXX, Sandia National Laboratories, Albuquerque, NM (in prep.).

Bechthold, W., Smailos, E., Heusermann, S., Bollingerfehr, T., Bazargan Sabet, B., Rothfuchs, T., Kamlot, P., Grupa, J., Olivella, S., and Hansen, F.D. 2004. Backfilling and Sealing of Underground Repositories for Radioactive Waste in Salt (BAMBUS II Project) : final report. European Commission: Directorate General for Research.

Edwards, H.C., & Stewart, J.R. 2001. SIERRA: A Software Environment for Developing Complex Multi-Physics Applications. In K.J. Bathe (ed.), *First MIT Conference on Computational Fluid and Solid Mechanics*. Amsterdam: Elsevier.

Freeze, G., Argüello, J.G., Howard, R., McNeish, J., Schultz, P.A., & Wang, Y. 2010. Challenge Problem and Milestones for: Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Integrated Performance and Safety Codes (IPSC). SAND2010-7175, Sandia National Laboratories. Albuquerque, NM.

Freeze, G., Argüello, J.G., Bouchard, J., Criscenti, L., Dewers, T., Edwards, H.C., Sassani, D., Schultz, P.A., & Wang, Y. 2011. Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Integrated Performance and Safety Codes (IPSC): FY10 Development and Integration. SAND2011-0845, Sandia National Laboratories. Albuquerque, NM.

Krieg, R.D. 1984. Reference Stratigraphy and Rock Properties for the Waste Isolation Pilot Plant (WIPP) Project. SAND83-1908, Sandia National Laboratories, Albuquerque, NM.

Matalucci, R.V., Christensen, C.L., Hunter, T.O., Molecke, M.A., & Munson, D.E. 1984. Waste Isolation Pilot Plant (WIPP) Research and Development Program: In Situ Testing Plan, March 1982. SAND81-2628, Sandia National Laboratories, Albuquerque, NM.

Morgan, H.S., Krieg, R.D., & Matalucci, R.V, 1981. Comparative Analysis of Nine Structural Codes Used in the Second WIPP Benchmark Problem. SAND81-1389, Sandia National Laboratories, Albuquerque, NM.

Munson, D.E. 1979. Preliminary Deformation-Mechanism Map for Salt (with Application to WIPP). SAND70-0079, Sandia National Laboratories, Albuquerque, NM.

Munson, D.E. & Dawson, P.R. 1979. Constitutive Model for the Low Temperature Creep of Salt (With Application to WIPP). SAND79-1853, Sandia National Laboratories, Albuquerque, NM.

Munson, D.E. & Dawson, P.R. 1982. A Transient Creep Model for Salt during Stress Loading and Unloading. SAND82-0962, Sandia National Laboratories, Albuquerque, NM.

Munson, D.E. & Dawson, P.R. 1984. Salt Constitutive Modeling using Mechanism Maps. *Proc. 1st International Conference on the Mechanical Behavior of Salt*, Clausthal-Zellerfeld: Trans Tech Publications.

Munson, D.E., DeVries, K.L., & Callahan, G.D. 1990a. Comparison of calculations and in situ results for a large, heated test room at the Waste Isolation Pilot Plant (WIPP). In Hustrulid & Johnson (ed.), *Rock Mechanics Contributions and Challenges, Proc. 31st U. S. Symposium on Rock Mechanics*. Rotterdam: Balkema.

Munson, D.E., Fossum, A.F., & Senseny, P.E. 1989. Advances in Resolution of Discrepancies between Predicted and Measured in Situ WIPP Room Closures. SAND88-2948, Sandia National Laboratories, Albuquerque, NM.

Munson, D.E., Jones, R.L., Hoag, D.L., & Ball, J.R. 1988. Mining Development Test (Room D): In Situ Data Report (March 1984 - May 1988) Waste Isolation Pilot Plant (WIPP) Thermal/Structural Interactions Program. SAND88-1460, Sandia National Laboratories, Albuquerque, NM.

Munson, D.E., Jones, R.L., Ball, J.R., Clancy, R.M., Hoag, D.L., & Petney, S.V. 1990b. Overtest for Simulated Defense High-Level Waste (Room B): In Situ Data Report (May 1984 - February 1988) Waste Isolation Pilot Plant (WIPP) Thermal/Structural Interactions Program. SAND89-2671, Sandia National Laboratories, Albuquerque, NM.

Notz, P.K., Subia, S.R., Hopkins, M.M., Moffat, H.K., & Noble D.R. 2007. Aria 1.5: User Manual. SAND2007-2734, Sandia National Laboratories, Albuquerque, NM.

SIERRA Solid Mechanics Team. 2010. Adagio 4.18 User's Guide. SAND2010-6313, Sandia National Laboratories, Albuquerque, NM.

Stone, C.M., Holland, J.F., Bean, J.E., & Argüello, J.G. 2010. Coupled Thermal- Mechanical Analyses of a Generic Salt Repository for High-Level Waste (ARMA-10-180). *Proc. American Rock Mechanics Association (ARMA) 44th US Rock Mechanics Symposium, 27-30 June 2010*. Salt Lake City: American Rock Mechanics Association.

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 Aria_to_Adagio`" 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                                  #
```

```
#                 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

  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

  ################################################
  ################ GLOBAL CONSTANTS ##############
  ################################################

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

  ################################################
  ############# FUNCTION DEFINITIONS #############
  ################################################
  Begin definition for function DHLW_power_flux_function
    Abscissa = time # [second]
    Ordinate = DHLW_power_flux # [watt (Nm/s)]/(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 [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]
            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 = 41.93926667 # 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)
                      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
                         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

# 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 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
        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

     ################################################
     ################## 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 ###############
        ################################################

        EQ Energy for Temperature        On All_blocks Using Q1 with Lumped_Mass DIFF
#SRC
        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 * (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

        ################################################
        ############## 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
           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
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
```

```
      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
#                             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 = 1314871.92 # Every 0.5*Months
   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

    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

################################################
###### 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
#     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  -0.14  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 F: SIERRA MECHANICS OPERTORS 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

APPENDIX G: HEATED ROOM COUPLED CALCULATION #2 (ENCLOSURE RADIATION METHOD) INPUT DECK

```
#-----------------------------------------------------------------------#
#     directory : /scratch/jsrath/NEAMS/roomb/coupled/simu1001
#          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
```

```
  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

  ################################################
  ################ GLOBAL CONSTANTS ##############
  ################################################

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

  ################################################
  ############# FUNCTION DEFINITIONS #############
  ################################################

  Begin definition for function DHLW_power_flux_function
    Abscissa = time # [second]
    Ordinate = DHLW_power_flux # [watt (Nm/s)]/(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 [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]
            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 = 41.93926667 # 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)
                     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
                         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

#
# 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
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 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 ###############
        ################################################

        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)
##      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")
##      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

        ################################################
        ############# 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
            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
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
#                             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 = 1314871.92 # Every 0.5*Months
   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

    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

   ################################################
   ###### 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
#     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  -0.14  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                          #
```

```
#                              = 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

  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 \#
                          319.20 321.50 323.40 324.60 325.20 \#
                          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 DHLW_power_flux_function
    Abscissa = time # [second]
    Ordinate = DHLW_power_flux # [watt (Nm/s)]/(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 [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]
             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 = 41.93926667 # 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)
                      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
                        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


  ################################################
```

```
  ############## 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
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

        ################################################
        ############ GOVERNING EQUATIONS ###############
        ################################################
```

```
        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)
##      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")
##      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
```

```
##################################################
######## 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
   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
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
```

```
#                              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 = 1314871.92 # Every 0.5*Months
   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

    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

################################################
###### 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
#           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  -0.14  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:

```
#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,
//                R.M. Clancy, D.L. Hoag, and S. V. Petney.
//                "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
Office of Fuel Cycle Research and Development
Attn: Jeffrey R Williams
NE-52/Forrestal Building
1000 Independence Ave. SW
Washington DC 20585

3 US Department of Energy
Attn: William Boyle
Prasad Nair
Tim Gunter
DOE-NE
232 Energy Way
North Las Vegas, NV 89030

1 Waste Isolation Pilot Plant
Attn: Roger Nelson
U.S. Department of Energy
4021 National Parks Highway
Carlsbad, NM 88220

Laboratories/Corporations

2 Argonne National Laboratory
Attn: M. Nutt
9700 S. Cass Avenue
Argonne, IL 60439

1 Los Alamos National Laboratory
Attn: Ned Elkins
115 N. Main
Carlsbad, NM 88221

1 Chandrika Manepally
Center for Nuclear Waste Regulatory Analyses
Geosciences and Engineering Division
Southwest Research Institute
6220 Culebra Road
San Antonio, TX 78238

Foreign Addresses

1 Commission nationale d'Évaluation (CNE)
Attn: Prof Pierre Berest
39-43, quai André Citroën
FR – 75015 Paris
France

2 NRG Petten – Dept. of Radiation & Environment
Attn: Dr Jaap Hart
Dr T.J. Schröder
P.O. Box 25
NL – 1755 ZG Petten
Netherlands

2 Institut für Gebirgsmechanik GmbH
Attn: Dr Wolfgang Minkley
Dr Till Popp
Friederikenstrasse 60
DE – 4279 Leipzig
Germany

2 DBE Technology GmbH
Attn: Dr Enrique Biurrun
Dr Nina Müller-Hoppe
Eschenstrasse 55
DE – 31224 Peine
Germany

1 Forschungszentrum Karlsruhe (FZK) GmbH
Attn: Mrs Alexandra Pudewills
Institut für Nukleare Entsorgung (INE)
Weberstrasse 5
DE – 76021 Karlsruhe
Germany

2 Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH - Final Repository Safety Research Division
Attn: Mr Tilmann Rothfuchs
Mr Klaus Wieczorek
Theodor-Heuss-Strasse 4
DE – 38122 Braunschweig
Germany

1 Forschungszentrum Karlsruhe (FZK) GmbH
(PTKA-WTE)
Attn: Dr Walter Steininger
Postfach 3640
DE – 76344 Eggenstein-Leopoldshafen
Germany

1 Clausthal University of Technology
Institut for Mineral and Waste Processing, Waste Disposal and Geomechanics
Attn: Mr Ralf WOLTERS
Adolph-Roemer-Straße 2a
DE – 38678 Clausthal-Zellerfeld
GERMANY

Internal

1	MS0372	J. G. Argüello	01525
1	MS0372	J. F. Holland	01525
1	MS0701	M. C. Walck	06900
1	MS0747	D. J. Clayton	06223
1	MS0751	F. D. Hansen	06910
1	MS0751	B.Y. Park	06914
41	MS0828	J.S. Rath	01525
1	MS0840	J. Pott	01525
1	MS1370	R. J. MacKinnon	06224
1	MS0899	Technical Library	09536 (electronic copy)


Sandia National Laboratories