Two problems to benchmark numerical codes for use in potential HLW salt repositories

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ABSTRACT: The assurance of a HLW repository's performance and safety, for the required period of performance, depends on numerical predictions of long-term repository behavior. As a consequence, all aspects of the computational models used to predict the long-term behavior must be examined for adequacy. This includes the computational software used to solve the discretized mathematical equations that represent the geomechanics in the computational models. One way, and perhaps among the best, to evaluate the overall computational software used to solve complex problems with many interacting nonlinearities, such as found in the response of a potential HLW repository in rock salt, is by the use of benchmark calculations whereby identically-defined parallel calculations are performed by two or more groups using independent but comparable capabilities. In this paper, the detailed definitions of two benchmark problems are presented that are consistent with idealizations of two WIPP in-situ full-scale underground experiments – WIPP Rooms B & D. It is hoped that the benchmark problems defined here will be useful to the salt community at large and allow others to benefit from their availability. These problems, or ones similar to these, can be used to assess the current generation of computational software available for modeling potential rock salt repositories.

1 INRODUCTION

For the geologic disposal of nuclear wastes there are several key factors in the development of a disposal repository that are needed to assure adequate containment and isolation of the radioactive wastes: (1) a sound design of the system; (2) validated computational models and tools to permit crafting system designs with confidence; and (3) acceptable techniques for evaluating (assessing) the design's performance by methods know to be valid (WMTD 1985). The second item above, on computational models and tools, will be the focus of this work. Specifically, how the use of benchmarking of the computational tools can help provide confidence in their validity for use on potential HLW salt repositories. Paramount to this is the importance of a careful and complete definition of the benchmark problems for use in the process.

The assurance of a HLW repository's performance and safety, for the required period of performance, depends on numerical predictions of long-term repository behavior. As a consequence, all aspects of the computational models must be examined for adequacy. This includes the computational software used to solve the discretized mathematical equations that represent the geomechanics in the computational models. Typically such computational software can be considered to include two major components: a numerical solution technique that solves the discretized equations over space and time; and the numerical implementation of constitutive models that are used to represent the geo-materials' behavior. One way, and perhaps among the best, to evaluate the overall computational software used to solve complex problems with many interacting nonlinearities, such as found in the thermo-mechanical response of a potential HLW repository in rock salt, is by the use of benchmark calculations whereby identically-defined parallel calculations are performed by two or more groups using independent but comparable capabilities.

Benchmarking activities have been undertaken by Sandia National Laboratories (SNL) in the past under the auspices of the Waste Isolation Pilot Plant (WIPP) and were very valuable exercises that provided an excellent assessment of the computational capability available at the time (Wayland & Bertholf 1980, Krieg et al. 1980, Morgan et al. 1987). They also provided invaluable information on how benchmark problems should be formulated and carried-out to maximize their benefit. However, in those previous exercises, the problems consisted only of well-defined boundary-value problems because development of WIPP was in its earliest stages. Since then, several large-scale in-situ experiments

were undertaken and completed at the WIPP, in the early to mid-1980's, to provide data on the creep response of the underground excavations under isothermal and heated conditions. WIPP was eventually licensed as the only repository in the U.S. for the disposal of transuranic (TRU) nuclear waste.

In this paper, the detailed definitions of two bedded salt benchmark problems are presented that are consistent with idealizations of two WIPP in-situ full-scale underground experiments – WIPP Rooms B & D. In our earlier efforts at trying to duplicate the "legacy calculations" of Munson (1997) (see Section 3), it was difficult to determine what assumptions and discretizations had been used in the various calculations that led to the final results documented in that article because some of the details of the calculations were missing. In this article we intend to provide as much detail as necessary, in a single document, for the benchmark calculations to be performed by any interested party. It is hoped that the benchmark problems defined here will be useful to the salt community at large and allow others to benefit from their availability. These problems, or ones similar to these, can be used to assess the current generation of computational software available for modeling potential rock salt repositories. Unlike in the previous benchmark exercises noted above, these benchmarking problems can be used to do code-code comparisons and also to do comparisons of code results to the full-scale experimental data that is available from the tests (Munson et al. 1988, 1990a). Select results to one of the defined benchmark problems computed with Sandia's current generation computational code suite, SIERRA Mechanics, will be presented and then compared to results that arise if various changes are made to the problem definition. This will help elucidate features of importance necessary for appropriately capturing the underground behavior of rooms in bedded salt and underscore why a detailed description of the problem is necessary in a benchmarking exercise.

2 TWO BENCHMARK PROBLEMS

Several full-scale in-situ experiments were fielded at the WIPP in the early 1980's (Matalucci 1987). Among these thermal/structural interactions (TSI) experiments were the Mining Development Test (Room D) and the Overtest for Simulated Defense High-Level Waste (Room B).

The first, Room D, was an "experiment of opportunity" (Munson et al. 1988) because the room was, initially, only intended to provide ventilation during construction of the other planned tests. However, because it had the same dimensions as other actual test rooms (e.g., Room B), it provided an opportunity to develop mining, instrumentation, and data acquisition methods at an early stage of the project. This was an isothermal room.

The second, Room B, was designed to distinguish how the host rock and the disposal room would respond to the effects of high heat. Specifically, its objectives were to determine room closure rate and heat transfer; to validate predictive techniques; and to evaluate the long-term effects of heat and room closure. In short it was an accelerated test that accentuated thermal loading and accelerated room closure and rock failure modes by increased deformation due to hastened creep (Munson et al. 1990a).

Except for the heat load, in Room B, both rooms were essentially identical. In addition to being the same dimensions, Rooms D and B: were located in the same general area of WIPP; were relatively isolated from other workings; were located at the same horizon and thus in the same vertical stratigraphic location; and both rooms were extensively instrumented. The comprehensive datasets for both rooms were archived and are available, thereby making these rooms well-suited for use in benchmarking.

The remainder of this section serves to document computational idealizations of these tests in one place and with sufficient detail to allow interested parties to use these as benchmark problems in the future. Idealizations similar to these are currently being used in a U.S.-German Joint Project aimed at benchmarking of advanced rock salt constitutive models and performance of numerical simulations (Hampel et al. 2013).

2.1 *Room D*

Room D was a 5.5 m by 5.5 m square room, in cross-section, that was mined at a depth of approximately 650 m (Clay G lies 650.45 m) below the ground surface in a bedded salt deposit that is laterally extensive and with an approximate thickness of 600 m. The evaporite beds are predominantly clean salt or argillaceous salt that are separated by thin interbeds of clay and anhydrite. Occasionally there may be anhydrite and polyhalite layers up to 4 m thick. Excavation of the room began on March 14, 1984 and ended on April 14, 1984. Additional details of the experiment can be found in the Room D data report (Munson et al. 1988) that presents the structural data acquired from both temporary and permanent gauges from March 1984 through May 1988.

The detailed stratigraphy 50 m above and below the room is shown in Figure 1, which also constitutes the idealized configuration of the Room D and Room B mechanical models with appropriate boundary conditions. This represents a plane-strain idealization of the room (half-room because of symmetry) that can be used to model the room response at the central portion of the 93.3 m long room.

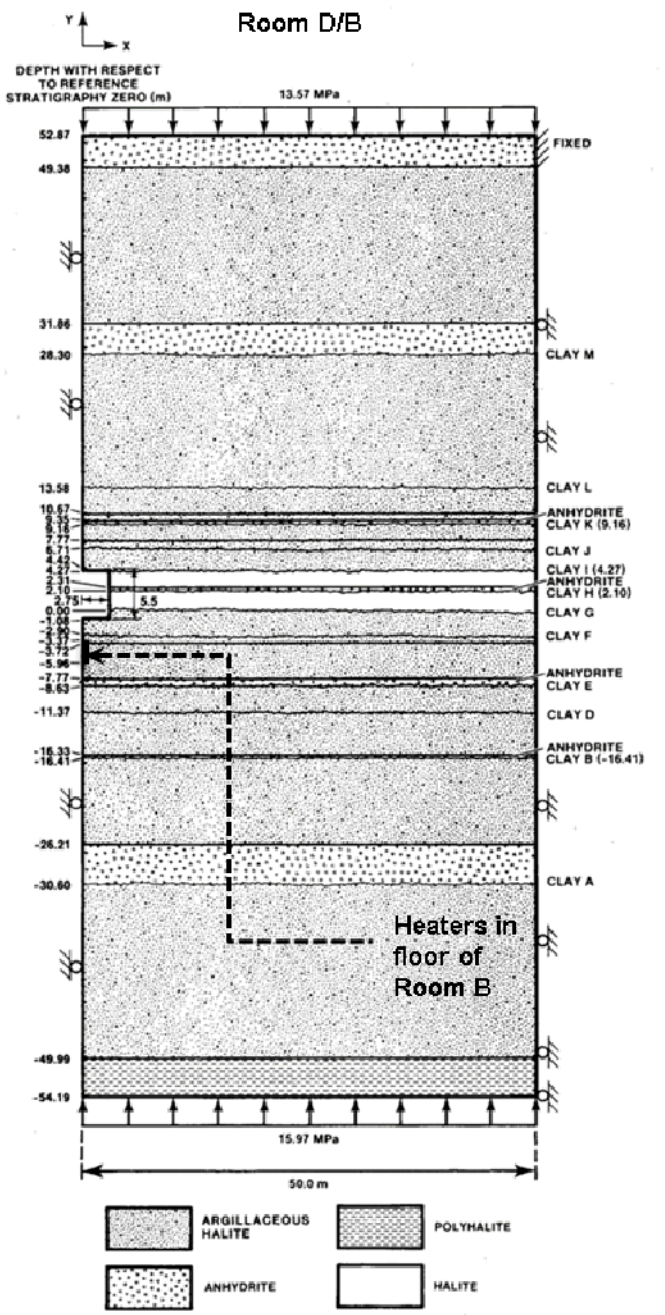

Figure 1. Idealized mechanical configuration of both Room D & B with boundary conditions.

The boundary conditions are such that the top has an applied traction of 13.57 MPa that accounts for the weight of the overburden. The bottom has a 15.97 MPa traction that accounts for the weight of the configuration and the presence of the room. The left side constitutes a plane of symmetry, while the right side constitutes a far-field boundary that was sufficiently removed (50 m) to preclude its affecting the room response for the simulation period. Both the left and right boundaries are restrained from moving horizontally (X-direction), and the right boundary of the uppermost anhydrite layer is also restrained against vertical movement (Y-direction) to prevent rigid-body motion in the numerical codes. In addition, the nine clay seams nearest to the room were assumed to be active (clays D-L) and were included in the model as sliding surfaces.

The initial stress in the configuration was assumed to be lithostatic (isotropic) and increased linearly from top to bottom with depth. The configuration was taken to be at a constant temperature of 300 °K and its average density was 2300 kg/m^3. The acceleration of gravity was taken as 9.79 m/s^2.

2.2 *Room B*

As previously mentioned, this room was identical in cross-section and length to Room D. However, Room B was excavated from May 4, 1984 to June 3, 1984. This room had electrically heated canisters placed in evenly-spaced boreholes in the floor along the room centerline. The heaters were nominally 0.30 m in diameter by 3.0 m long (with a heated length of 2.59 m), and the emplacement boreholes were 0.41 m in diameter by 4.9 m deep. Each of the heaters had a power output of 1.8 kW. These were spaced at 1.52 m centers to provide an equivalent linear heat load of 1.18 kW/m over the central 41.2 m of the room. At both ends of the room there were additional waste package performance (WPP) and guard heaters installed, with the heater location and power selected to compensate for the "end effects" of the finite length of the heated section of the room. In addition, there were also insulated doors installed at both ends of the room to mitigate thermal losses due to mine ventilation air circulating past the entries. Nonetheless heat losses did occur through the insulated doors (Munson et al. 1990a) and need to be accounted for in the model.

The room operated in an unheated condition until April 23, 1985 and served to give a baseline response for comparison to other similar rooms (e.g., Room D). When the heaters were activated, the insulated doors at the ends of the room were closed and access to the room was restricted to minimize room heat loss. On February 7, 1988 the experiment was interrupted to permit ventilation and subsequent recovery of the WPP heater tests from the room. This interruption occurred about 1374 days after the start of room excavation, 1020 of which were heated days. Additional details of the experiment can be found in the Room B data report (Munson et al. 1990a) that presents the structural and thermal data acquired from May 1984 through February 1988.

The mechanical boundary conditions were identical to those of Room D, described earlier. In the thermal model of Room B, all boundaries except for the room periphery were assumed to be adiabatic. The far-field boundaries (as was the case for the mechanical portion) were sufficiently removed to preclude them from affecting the response of the room throughout the simulation period. The entire formation was prescribed to be at an initial temperature of 300 °K. The actual room area was assumed to

consist of an "equivalent thermal material" (ETM) that was included only in the thermal mesh. The ETM had a high constant thermal conductivity and a high thermal diffusivity, that simulates the convective and radiative transfer in the room by an equivalent conduction. Newton's Law of Cooling was used to represent the convective heat losses from the room periphery.

2.3 *Constitutive Models & Parameters*

While the previous two sub-sections have covered the details of the boundary and initial conditions used to define the two room models and would be consistent with the information needed by any numerical code, the definition of the constitutive models for salt and the parameters specifically used by SNL in our numerical codes for the two calculations are documented here. It is anticipated that other users would bring different numerical tools to bear on these problems that may involve the use of different constitutive models and parameters. Those users would need to have appropriate laboratory experimental data to define their constitutive models.

2.3.1 *Mechanical*

The salt was modeled with the Multi-mechanism Deformation (MD) Creep Model. 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. Because the MD model is well-described elsewhere (e.g., Munson et al. 1989a, Munson 1997), it will not be repeated here. However, the MD Creep Model properties for clean and argillaceous salt that were used in these calculations are given in Table 1. As noted, there are two types of salt properties included in the table, those for clean salt and those for argillaceous salt. Most of the parameters are the same for both salts but there are some parameters that differ for the argillaceous salt (A_1, B_1, A_2, B_2, K_0, & α).

The anhydrite and polyhalite can be modeled with an elastic perfectly-plastic Drucker-Prager criterion:

$$F = \sqrt{J_2} + aI_1 - C \qquad (1)$$

where $I_1=\sigma_{kk}$; $J_2=S_{ij}S_{ji}/2$; and a & C are material constants. The parameters for the two materials are shown in Table 2.

As previously mentioned, the clay seams were modeled as sliding surfaces, and they were assumed to be infinitely thin. Their response was modeled with a Mohr-Coulomb model: $\tau=\mu\sigma_n$, where σ_n is the normal stress across the surface and μ is the coefficient of friction. The coefficient of friction was taken as 0.2 for all sliding surfaces in the calculations.

Table 1. MD creep model parameters for clean and argillaceous salt (different values for argillaceous salt in parentheses).

	Parameters		Units	Salt
Salt 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		6.086×10^{6} (8.998×10^{6})
		A_2		9.672×10^{12} (1.314×10^{13})
		B_2		3.042×10^{-2} (4.289×10^{-2})
	Activation Energies	Q_1	cal/mole	25,000
		Q_2		10,000
	Universal Gas Constant	R	cal/mole-°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} (1.783×10^{6})
		c	$°K^{-1}$	9.198×10^{-3}
	Constants for work-hardening parameters	α	–	-17.37 (-14.96)
		β		-7.738
	Recovery parameter	δ	–	0.58

Table 2. Drucker-Prager parameters used for anhydrite and polyhalite.

Material	E (MPa)	ν	a	C (MPa)
Anhydrite	75,100	0.35	0.450	1.35
Polyhalite	55,300	0.36	0.473	1.42

2.3.2 *Thermal*

Heat transfer through the salt, anhydrite, and polyhalite was modeled with a nonlinear thermal conductivity of the form:

$$\lambda = \lambda_{300}(300 / \mathrm{T})^{\gamma} \quad (2)$$

where λ is the thermal conductivity, T is the absolute temperature in Kelvin, and λ_{300} & γ are material constants. The various parameters are given in Table 3 and include: C_P (the specific heat), α (the coefficient of linear thermal expansion), and ρ (the material density).

Table 3. Thermal modeling parameters for the various materials in the model.

Material	C_P J/(kg-K)	α K^{-1}	λ_{300} W/(m-K)	γ	ρ kg/m^3
Salt	862	45×10^{-6}	5.4	1.14	2,300
Anhydrite	733	20×10^{-6}	4.7	1.15	2,300
Polyhalite	890	24×10^{-6}	1.4	0.35	2,300
ETM	1000	-	50.0	0.00	1

As mentioned previously, thermal loss from the room was modeled by a convective boundary at the room peripheral surfaces using Newton's Law of cooling:

$$\bar{q}\cdot\bar{n} = h(T - 300) \quad (3)$$

Where $\bar{q}$ is the thermal flux vector, $\bar{n}$ is the outward normal unit vector, h is the convective heat transfer coefficient, and T is the surface temperature. This boundary acts as a heat sink as soon as the room temperature exceeds the initial 300 °K temperature. The rate of heat loss increases as the room surface temperature rises. During the legacy calculations, the convective heat transfer coefficient, h, was unknown, so it was adjusted (prior to the mechanical calculations) until a "suitable value (0.51 W/m^2-K) was determined to give agreement with the measured temperatures" (Munson et al. 1990b).

3 COMPUTED RESULTS FOR ROOM D

Select computed result from the Room D benchmark problem, as defined above, will be described and discussed in this section. In preparation for the WIPP Room B and D benchmarking exercise that is to be undertaken by all partners of the U.S.-German Joint Project mentioned earlier, the author performed additional analyses on Room D that will help guide the final specification and description of the benchmark problems.

However, to put the current efforts in the proper context it is necessary to provide some background to the earlier numerical modeling work performed by Sandia on these two rooms with legacy computational capabilities in the mid-1980s to early-1990s timeframe, prior to WIPP licensing (Munson 1997). Those analyses were performed using the mechanical SPECTROM-32 computer code (Callahan, et al. 1990) with the MD Creep model (Munson and Dawson 1979, 1982, 1984; Munson et al. 1989a) and the thermal SPECTROM-41 computer code (Svalstad 1989), for the heated room case. Hereafter we will refer to these, collectively, as the "legacy calculations."

3.1 *Legacy Computational Capabilities*

In the mid-1980s to early-1990s, the state of computing was such that single-processor (central processing unit [CPU]) computers with low processing speed and limited memory (compared to today) were the norm for the thermo-mechanical numerical analysis work typical to salt repositories. Furthermore, although early three-dimensional computational capability was starting to be introduced, two-dimensional computer programs for performing those creep thermo-mechanical calculations, under axisymmetric or plane strain conditions, were the norm.

Because of the aforementioned constraints (state of computers and codes) in performing salt creep repository thermo-mechanical calculations at the time, the analyst had to make some tradeoffs between his desire for fidelity in the model, in terms of refinement, and his desire to get a solution. If the mesh refinement of the model was too fine, it would either not fit into random access memory (RAM) and/or it would take too long to run on the computer – in some cases, weeks or months.

Mesh refinement of a model has always been an important consideration when performing a numerical simulation and it was well-known even at the time that sufficient refinement was needed to get a converged solution, because too-coarse of a mesh would produce results that were too stiff relative to one with sufficient refinement. All too often, however, the refinement of the model would be sacrificed in order to get a solution within a reasonable amount of time (i.e., multiple days, rather than multiple weeks or months). Although it would now be considered good-practice, performing a mesh convergence study in the mid-1980s to early-1990s was not the norm and, in fact, may not have been possible for disposal room thermo-mechanical problems of that day.

3.2 *30 Years of Advancements*

The ensuing thirty years since those early days have led to significant advancements, and these have resulted in efficient frameworks and enabling tools & infrastructure to produce a new generation of high-fidelity simulation tools that incorporate the advances in both hardware (computers) and software (algorithms and computer programs). In 2014, "multi-core" workstations, moderately parallel clusters, and/or massively parallel computers are widely available. The processors in those machines are significantly faster than those available during the time

of the legacy calculations and are likely to be "multicore" (a single chip that contains more than one CPU). Furthermore, the price of memory has dropped significantly, as well, and ample memory in those machines is the norm. For example, the author has a sixteen core workstation with 64 GB of RAM that he uses for small repository problems. For mid-size problems there is access to several compute clusters ranging from 40 up to 120 cores each and 1–2 TB of RAM each. For truly large problems there is also access to the large institutional massively parallel machines with thousands of processors and plentiful memory.

In addition to the advancements in hardware over the past thirty years, algorithms and computational simulation software have likewise seen significant developments and improvements. The current generation of computer codes is capable of handling fully three-dimensional single-physics or, if needed, multi-physics problems. Sophisticated algorithms and frameworks are in-place to allow said software to easily use from one to thousands of CPUs for solving repository thermo-mechanical creep problems. One such example is the SNL SIERRA Mechanics code suite (Edwards and Stewart 2001). The goal of this suite is the 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.).

With the hardware and software capability available at present, there should be no practical limit on the refinement of the model in the conduct of a thermo-mechanical salt creep disposal room simulation. Additional refinement still incurs more cost, but the analyst can typically bring additional processors to bear on the problem at hand to avoid the extremely long times that would have plagued an analyst in the time of the legacy calculations. Therefore, it is currently possible to solve a creep thermo-mechanical problem at the appropriate refinement level – something not possible in the mid-1980s to early 1990s.

3.3 *Current Efforts*

The capability to model waste repositories and salt creep is a relatively recent addition to SIERRA Mechanics. Consequently, data from the same WIPP Rooms D and B are currently being used in an effort aimed at assessing the Sierra Mechanics code suite for this class of problems. Up to now, work has focused on trying to duplicate the results from the legacy calculations of Munson and co-workers (Argüello & Rath 2012, 2013). It should be noted that the work reported in the Munson (1997) article actually began in the mid-1980s with the first results of WIPP Room D results, using an updated MD creep model, reported by Munson et al. (1989a). In addition, this latter report incorporated changes in the stratigraphy in the model of the WIPP rooms that departed from earlier interpretations of the stratigraphy as documented by Krieg (1984). Additional thermo-mechanical simulation work on the various WIPP room models continued throughout the 1980s up to the mid-1990s (Munson et al. 1989b, 1990b, and Munson & DeVries 1991) and culminated in the Munson (1997) article. In trying to duplicate the results of the legacy calculations on WIPP Rooms D and B, we have been using a model of the rooms with mesh refinement comparable to what was used in the mid-1980s to early-1990s. Determining what sort of mesh refinement was used in the actual Room D and B legacy calculations of Munson and co-workers has not been possible because the size of the model(s) used and/or figures showing the mesh that was used are absent in the documentation of the various results.

However, the work of Morgan & Stone (1985) does provide such information on model size and was conducted in approximately the same time period. So, in lieu of no problem-size information from the legacy calculations documentation, a mesh similar to that of Morgan & Stone (1985) was used in the attempt to duplicate the legacy WIPP Room D calculations. This mesh, shown in Figure 2, is representative of the refinement used by analysts in the timeframe of the legacy calculations. This is also the mesh that has been transmitted to the German partners to aid in their setup of the problem. The mesh consists of 5,032 nodes and 2,184 hexahedral elements. The mesh is comprised of a single-element through the thickness to mimic the plane strain conditions of the legacy calculations with the three-dimensional SIERRA Mechanics code (it is only 3D capable). It also contains four element blocks that represent the four materials: clean salt, argillaceous salt, anhydrite, and polyhalite.

By current standards, this mesh is relatively coarse. However, the original goal of our current effort (Argüello & Rath 2012, 2013) was to attempt to duplicate the legacy calculations, so such a mesh refinement was consistent with that goal. Figure 3

shows the vertical closure results for Room D obtained with this "original" mesh. Two solid curves are shown. One representing a simulation in which an "all-salt" configuration was used and another in which the full stratigraphy shown in Figure 1 was used.

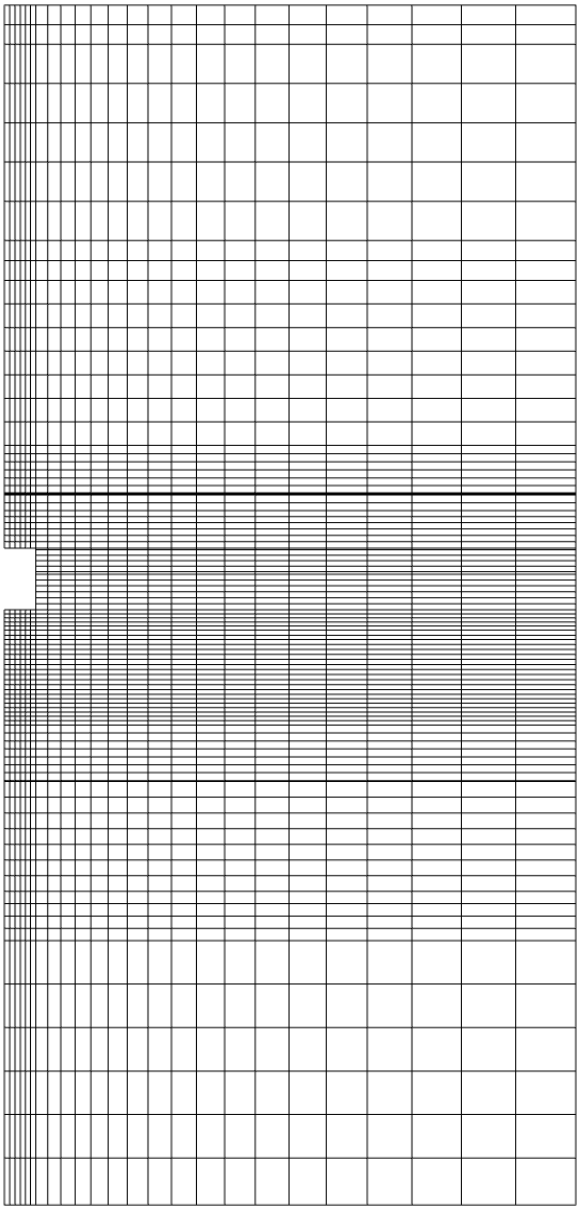

Figure 2. Coarse mesh used in the calculations.

By all-salt, it is meant that the clean salt and argillaceous salt layers are honored as such and use the material properties for each material as given in Table 1. However, the anhydrite and polyhalite layers were treated as if they were actually clean salt, again with the properties given in Table 1 for clean salt, as opposed to our earlier work (Argüello & Rath 2012) which treated both of the materials as argillaceous salt in Room D. Such an all-salt idealization appears to have been used in the earliest legacy calculations (Munson et al. 1989a) that looked at the response of WIPP Room D. As stated in (Munson et al. 1989a): "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 uninfluential in the calculational response, we did not include them in the calculation." Furthermore, later in the same report: "In the calculations, each of the layers in the stratigraphy of the calculational model have properties as defined in the previous section of the report" – only clean salt and argillaceous salt properties are defined in the referenced section. From the report, it is unclear which of the properties (clean salt or argillaceous salt) were used to represent the anhydrite and polyhalite in those early legacy calculations. Hence, we have chosen here to treat both of those materials as if they were clean salt. As seen in Figure 3, the computed vertical closure results with an all-salt stratigraphy for Room D are in very good agreement with the measurements up through the end of the 1100 day simulation time. This result is also consistent and comparable to the early legacy calculational results (see Figure 3.5 of Munson et al. 1989a).

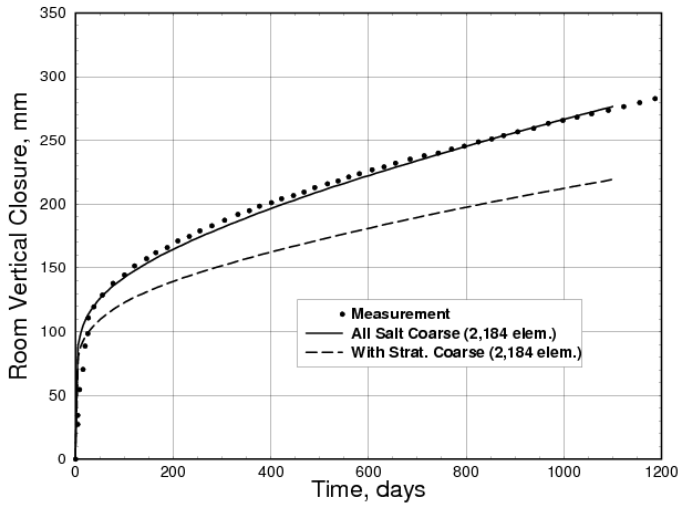

Figure 3. Computed vertical closure of Room D with coarse mesh compared to measured room vertical closure.

4 DEVIATIONS FROM ORIGINAL DEFINITION

In this section, we make various changes to the prescribed original problem definition (from Section 3) for Room D that might seem relatively inconsequential at first look, but that turn out to cause significant deviations in the computed response. First off, what does the use of the real full stratigraphy produce, in terms of vertical closure compared to treating the anhydrite and polyhalite as clean salt?

The full stratigraphy calculation now used distinctly different properties from salt for the anhydrite and polyhalite. It also used a different constitutive model for the representation of their behavior. In this case, the anhydrite and polyhalite were mod-

eled with the elastic, perfectly-plastic Drucker-Prager criterion defined earlier in Section 2 and used the properties for the two materials shown in Table 2. As seen in Figure 3, the computed vertical closure results with the full-stratigraphy for Room D lie significantly below the measured values throughout the simulation time. Although a difference in response was expected, it is perhaps larger than anticipated.

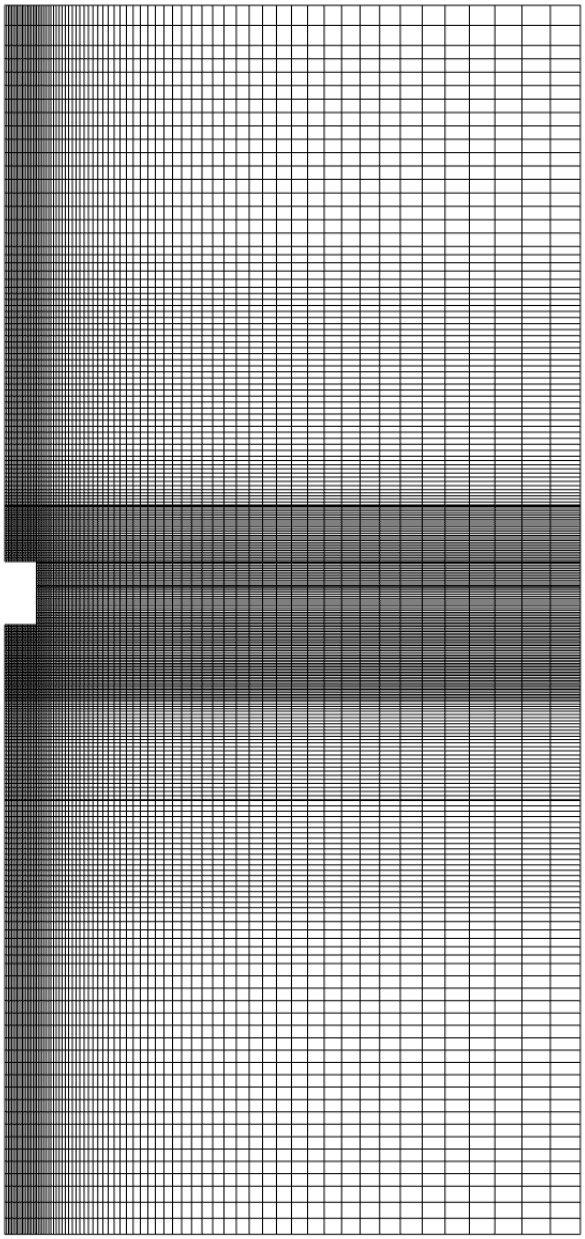

Figure 4. Refined mesh used in the new calculations.

The latest work in the current effort focusses on developing a benchmark problem definition for the U.S.-German Joint Project (Hampel et al. 2013). Because this problem will use state-of-the-art (SOA) constitutive models and SOA computational codes/resources, it was desirable to bring the entire model, including its mesh discretization, up to a level consistent with current practice, knowing that the original mesh was rather coarse. Figure 4 shows a mesh with a significantly increased level of refinement over the original coarse mesh. This finer mesh contains about eight times the refinement of the original mesh – 36,482 nodes and 17,298 hexahedral elements. Everything else in the model remained the same. Again, it should be re-iterated, that the use of an order-of-magnitude more elements (i.e., approximately this level of refinement) in the mid-1980s to early-1990s would have been prohibitive.

Figure 5 shows the Room D computed vertical closure with this more refined mesh for both the all-salt case and the full stratigraphy case. What can be seen in the figure for this refined mesh is that now the all-salt stratigraphy calculation over-estimates the measured closure. For the case with the full stratigraphy, the computed vertical closure curve still lies below the measured values, but is now closer than what was seen with the original coarse mesh in Figure 3. This is what would be expected for a computational problem in which the mesh is under-refined – a coarser mesh would provide answers that are too stiff and further refinement would soften (reduce the stiff behavior of) the response. As a consequence, the all-salt stratigraphy case and the full stratigraphy case are now bracketing the measured vertical closure of the room.

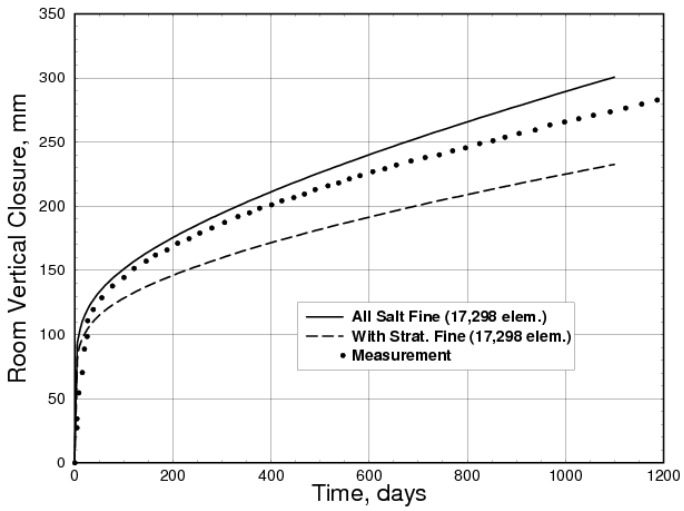

Figure 5. Computed vertical closure of Room D with refined mesh compared to measured room vertical closure.

By extension to what is seen in Figure 5, if a mesh of comparable refinement to the original coarse mesh was used in the legacy calculations, it too would have been under-refined. This would imply that in the legacy calculations (Munson 1997), the MD parameters along with other features in the model (e.g., coefficient of friction), would have been calibrated to match the tests using a relatively coarse mesh – albeit, a mesh that would have been quite reasonable at the time. Therefore, on the one hand, this remains an open question because the actual mesh used for the legacy calculations is unknown (not documented in any of the various articles per-

taining to the legacy calculations). On the other hand, this provides impetus for our work under the U.S.-German Joint Project as we analyze the two WIPP rooms under the benchmarking exercise and compare the responses from the various participants. The results of the benchmark exercise should allow us to address the question through the use of several state-of-the-art constitutive models and comparable capabilities to those of SNL that will be brought to bear on the two rooms. It further implies that a common refinement of the room model (perhaps finer even than shown) among the partners will likely be needed to be able to make appropriate comparisons between the results of the various partners participating in the benchmark.

It is worth noting that the previous WIPP benchmarking exercises (Wayland & Bertholf 1980, Krieg et al. 1980, Morgan et al. 1987) provided much information on how benchmark problems should be formulated and carried-out to maximize their benefit. However, it is rather curious that the issue of mesh refinement appears to have been relegated to the area of "code specific details," and the participants in those earlier exercises were allowed great latitude in choosing the level of refinement. As demonstrated here, the level of mesh refinement used in a problem can be very important and care should be taken to ensure that adequate refinement of the mesh is included in the specification of a benchmark problem.

5 SUMMARY & CONCLUSIONS

The detailed definitions of two benchmark problems are presented that are consistent with idealizations of two WIPP in-situ full-scale underground experiments – WIPP Rooms B & D. It is intended that the benchmark problems defined here will be useful to the salt community at large and allow others to benefit from their availability. These problems, or ones similar to these, can be used to assess the current generation of computational software available for modeling potential rock salt repositories.

A series of calculations has been completed for Room D using Sierra Mechanics and the MD Creep Model. These have addressed variations of the problem definition, from that of the original definition which used an all-salt stratigraphy to produce good agreement between the measured and computed vertical closure. The use of the full stratigraphy, with the use of the Drucker-Prager material model and properties for the anhydrite and polyhalite, produced a vertical closure of the room that was significantly smaller than the measured values when the original coarse mesh was used. This led to an investigation of the refinement of the mesh, as it was recognized that the original one was too coarse. With a mesh that is approximately an order of magnitude more refined, it was found that the measured vertical closure response of the room was now bracketed by the computed vertical closure response of an all-salt idealization and the full stratigraphy idealization. This suggests that the original mesh used in the legacy calculations of Munson (1997) may not have been sufficiently refined and that MD parameters and other features of the model (e.g., μ for clay seams) may have been calibrated to match the tests using a relatively coarse mesh – one that would have been acceptable at the time.

This remains an open question that provides impetus for our efforts under the U.S.-German Joint Project as we complete the benchmarking exercise and compare the responses from the various participants. Furthermore, it implies that a common relatively fine refinement of the room model among the partners will likely be needed to be able to make appropriate comparisons between the results of the various partners participating in the benchmark.

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