Results from the US-German Benchmark Initiative for FY14

Fuel Cycle Research & Development

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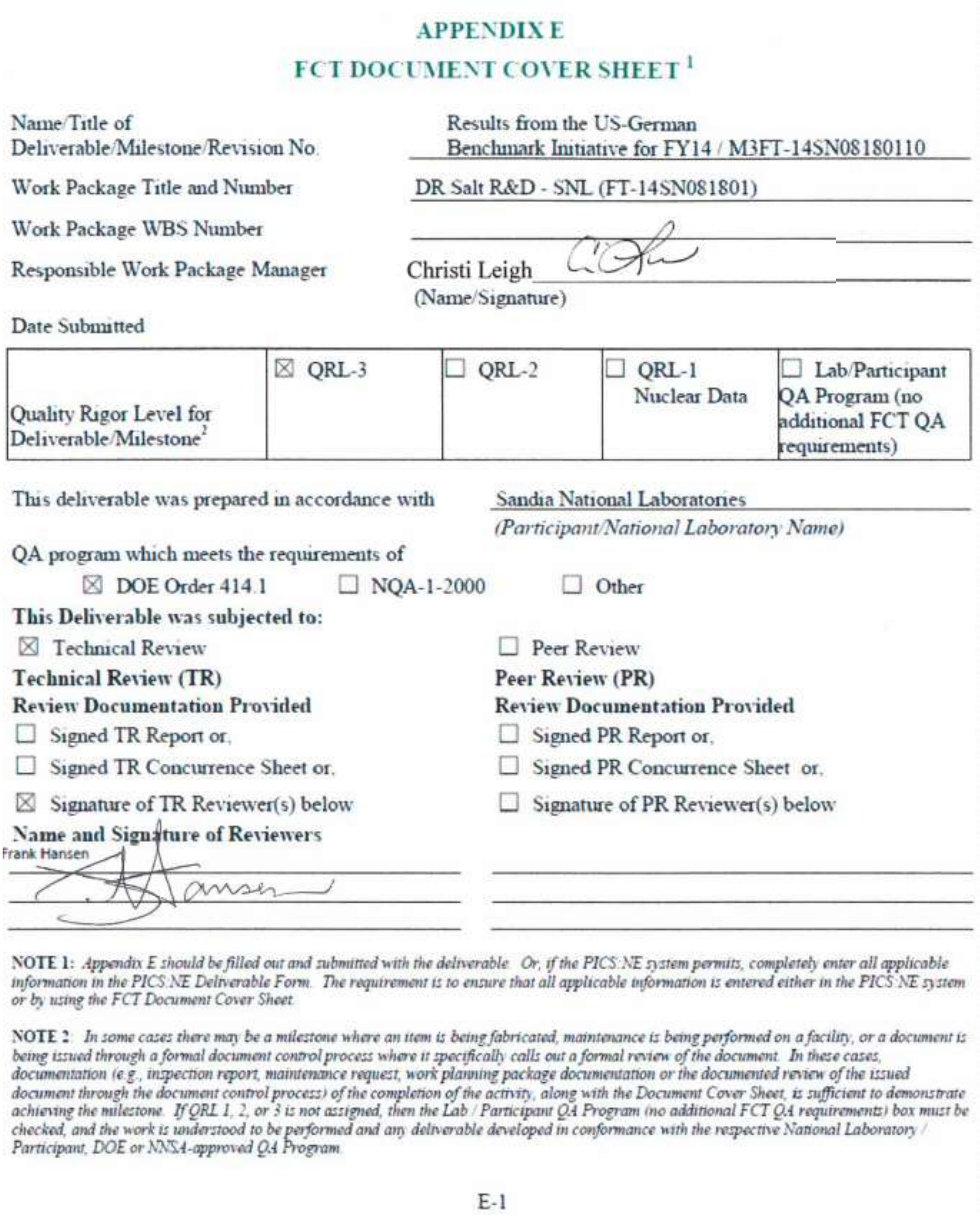

APPENDIX E

FCT DOCUMENT COVER SHEET [1]

Name/Title of Deliverable/Milestone/Revision No. Results from the US-German Benchmark Initiative for FY14 / M3FT-14SN08180110

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Responsible Work Package Manager Christi Leigh
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Quality Rigor Level for Deliverable/Milestone[2]	☒ QRL-3	☐ QRL-2	☐ QRL-1 Nuclear Data	☐ Lab/Participant QA Program (no additional FCT QA requirements)

This deliverable was prepared in accordance with Sandia National Laboratories
(Participant/National Laboratory Name)

QA program which meets the requirements of

☒ DOE Order 414.1 ☐ NQA-1-2000 ☐ Other

This Deliverable was subjected to:

☒ Technical Review	☐ Peer Review
Technical Review (TR)	**Peer Review (PR)**
Review Documentation Provided	**Review Documentation Provided**
☐ Signed TR Report or,	☐ Signed PR Report or,
☐ Signed TR Concurrence Sheet or,	☐ Signed PR Concurrence Sheet or,
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Name and Signature of Reviewers

Frank Hansen

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E-1

SUMMARY

Sandia recently joined the third phase of and is a contributing partner to a U.S.-German “Joint Project” entitled “Comparison of current constitutive models and simulation procedures on the basis of model calculations of the thermo-mechanical behavior and healing of rock salt.” The first goal of the project is to check the ability of numerical modeling tools to correctly describe the relevant deformation phenomena in rock salt under various influences. Achieving this goal will lead to increased confidence in the results of numerical simulations related to the secure storage of radioactive wastes in rock salt, thereby enhancing the acceptance of the results. These results may ultimately be used to make various assertions regarding both the stability analysis of an underground repository in salt during the operating phase and the long-term integrity of the geological barrier against the release of harmful substances into the biosphere in the post-operating phase. Among the numerical modeling tools are constitutive models that are used in computer simulations for the description of the thermal, mechanical, and hydraulic behavior of the host rock under various influences and for the long-term prediction of this behavior into the future.

A second goal of the project is to investigate and demonstrate the possibilities for further potential development and improvement of these constitutive models. This report summarizes the efforts undertaken during FY14 in support of these international benchmark calculations of field experiments.

ACKNOWLEDGMENTS

The author wishes to acknowledge John F. Holland, James E. Bean, and Jonathan S. Rath for their contributions to the various efforts during FY2014 and prior years. The dedication of this team, in the face of many challenges, has been outstanding! Special thanks also to Frank Hansen and Andrew Orrell (now with IAEA) for their support and encouragement in promoting this important international collaboration. 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.

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ACRONYMS

BfS	Bundesamt für Strahlenschutz
BGR	Bundesanstalt für Geowissenschaften und Rohstoffe
CDM	Composite Dilatancy Model
CPU	Central Processing Unit
DOE	Department of Energy
ERAM	Endlager für Radioaktive Abfälle Morsleben
FCR&D	Fuel Cycle Research & Development
GB	Giga-Byte
HFCP	Heated Free Convergence Probe
HLW	High-Level Waste
IFC	Isothermal Free Convergence
IfG	Institut für Gebirgsmechanik GmbH
IJRMMS	International Journal of Rock Mechanics and Mining Science
INE	Institut für Nukleare Entsorgungstechnik
KIT	Karlsruher Institut für Technologie
MD	Multi-mechanism Deformation
NE	Office of Nuclear Energy
NWTRB	Nuclear Waste Technical Review Board
RAM	Random Access Memory
SNF	Spent Nuclear Fuel
SOA	State-of-the-Art
TB	Terra-Byte
THM	Thermo-Hydrologic-Mechanical
TSI	Thermal/Structural Interactions
TUBS	Technische Universität Braunschweig
TUC	Technische Universität Clausthal
UFD	Used Fuels Disposition
US	United States
WIPP	Waste Isolation Pilot Plant

RESULTS FROM THE US-GERMAN BENCHMARK INITIATIVE FOR FY14

1. INTRODUCTION

This report serves to summarize and document work on the various activities related to the international benchmark calculations of field experiments undertaken in FY14. The activities include:

(1) Participation in and presentations at the Eleventh Joint Project III meeting held at IfG in Leipzig, Germany and the 4th US-German Workshop on Salt Repository Research, Design, and Operation held at the Hollywood Media Hotel in Berlin, Germany;

(2) Participation in and presentation in support of the Twelfth Joint Project III meeting at KIT, Karlsruhe, Germany;

(3) Transmittal of the WIPP Mining Development (Room D) coarse finite element mesh to the German partners and work on preliminary US-German Joint Project III WIPP benchmarking problems definition;

(4) Participation and presentations at various meetings, pertinent to the use of modeling for rock salt repositories, including: the Nuclear Waste Technical Review Board (NWTRB) meeting of March 19, 2014 in Albuquerque, New Mexico; the 48th US Rock / Geomechanics Symposium at University of Minnesota, Minneapolis, Minnesota; and the Used Fuels Disposition meeting in Las Vegas, Nevada

(5) Participation in the Thirteenth Joint Project III meeting at Sandia National Laboratories, Albuquerque, New Mexico; and

(6) Participation in and presentation at the 5th US-German Workshop on Salt Repository Research, Design, and Operations in Santa Fe, New Mexico.

An overarching effort, under these activities, has been to influence the international benchmarking work being conducted under the US-German Joint Project on "Comparison of Current Constitutive Models and Simulation Procedures on the Basis of Model Calculations of the Thermo-Mechanical Behavior and Healing of Rock Salt" (hereafter Joint Project III) by promoting the inclusion, in the benchmarking activities, of the high-quality in-situ room data available from the U.S. full-scale Thermal-Structural Interactions (TSI) experimental program undertaken at the WIPP (Munson et al. 1988, 1990a) in the early 1980s. This has resulted in the successful addition of WIPP Rooms D (isothermal) and B (heated) into the benchmarking effort of Joint Project III. The inclusion of WIPP Rooms D and B will help the international community exercise and hopefully demonstrate the applicability of the current state-of-the-art salt constitutive models to bedded salt. There is special interest, particularly, in the constitutive models for salt that have been advanced in the recent past (past decade) by the German scientific community. To date these German models have been exercised primarily on underground facilities in non-bedded (domal) salt. The following summarizes the various activities related to this milestone. Summaries of the international meetings in which the writer has participated are taken from meeting notes, materials presented at the meetings, and trip reports.

2. ELEVENTH JOINT PROJECT III MEETING AND THE 4th US-GERMAN WORKSHOP ON SALT REPOSITORY RESEARCH, DESIGN, AND OPERATION

These two events were held next to each other during the third week of September in Germany to facilitate travel for US participation. The Joint Project meeting was held, first, on Monday and was followed by the 4th US-German Workshop on Tuesday and Wednesday, followed by technical tours on Thursday and Friday.

Eleventh Joint Project III Meeting – The author attended the quarterly project meeting (workshop) of the US-German Joint Project III held at the Institut für Gebirgsmechanik GmbH (IfG) in Leipzig. The meeting was scheduled to precede the 4th US-German Workshop on Salt Repository Research, Design, and Operation that was held in Berlin from September 17-20th (including technical tours). The purpose of the meeting was to bring all of the partners up-to-date on the progress of the ongoing work since the last quarterly meeting. First off, because we were to report on the progress of Joint Project III to the more general and subsequent 4th US-German Workshop, Andreas Hampel (on the German side) and the writer (on the US side) gave a dry-run of their two-part presentation to the Joint Project III partners. This was followed by a presentation by Till Popp (IfG) related to the ongoing work on laboratory testing of WIPP salt core that had been provided to the German partners by the US. Questions with regard to humidity, distribution of polyhalite in the clean salt at WIPP, and differences in creep rate between 4" and 12" core were raised in this presentation. Another issue that was raised was that the long-held assertion, that WIPP salt creeps much faster than ASSE salt, was not seen in the testing of the clean WIPP salt by the Germans. It should be noted, however, that there has not yet been any testing of the Argillaceous salt samples that were sent to the Germans, so that this finding should be considered as a preliminary one at this point in time.

The next series of presentations were by Herchen (TUC) and Gunther (IfG) who talked about the ongoing work on rock salt "healing" laboratory tests and the numerical modeling of these tests. Herchen presented new calculations of the various healing tests that have been run with an updated "Lux-Wolters" model and Gunther also presented updates to the "Gunter-Salzer" model to be able to successfully capture the behavior of the tests. Herchen then talked about some new healing tests that TUC is running and how their apparatus has been modified to perform these new tests with better control and accuracy.

Thereafter, various presentations related to the progress on the Dammjoch (bulkhead) numerical modeling of damage and healing followed. Pudewills (KIT), Yildirim (Hannover), and Hampel presented the bulkhead results obtained with their respective models. There was also discussion on which results are to be compared among the partners and what variants of the analysis are to be completed.

In preparation for next year's start of the WIPP Rooms B & D calculations that the partners will perform, the writer was asked to provide a starting mesh for WIPP Room D to all the partners, as an action item. The next Joint Project III quarterly meeting was scheduled to be held in mid-January (16th-17th) 2014 in Karlsruhe, Germany.

4th US-German Workshop on Salt Repository Research, Design, and Operation – The author next traveled by train to Berlin with a subset of the Joint Project III participants to attend and present at the 4th US-German Workshop on Salt Repository Research, Design, and

Operation (Hansen, et al. 2013) that was held at the Hollywood Media Hotel in Berlin. This workshop dealt with broader repository-related issues such as: Selected Aspects of the Safety Case for Salt Disposal of HLW/SNF; Plugging and Sealing; Geochemical Issues; Rock/Salt Mechanics (THM-modeling); Repository Design and Operations; and Miscellaneous Important Issues. The writer co-presented, along with Andreas Hampel, on the status of the US-German Joint Project III ongoing work in the Rock/Salt Mechanics session. The presentation was entitled: “Status of the US-German Joint Project on ‘The Comparison of Current Constitutive Models . . .’” (SAND2013-7320C). He also participated in the discussions/interactions related to the more general issue of applicability of the results from the Joint Project to a potential repository sited in rock salt and addressed any questions related to the interfacing and coupling of the thermo-mechanical effects with other physics of importance in a repository setting (i.e., hydrological, chemical, etc. effects). In addition, he participated in technical tours to German repository sites that were associated with the 4th US-German Workshop as discussed next.

Following the Workshop, and in association with it, the writer participated in technical tours of the Morsleben Repository and the mining damage region Staßfurt. The Endlager für radioaktive Abfälle Morsleben (ERAM) or Radioactive Waste Repository Morsleben is a repository for low-level and intermediate-level radioactive waste and a former potash and rock salt mine in Saxony-Anhalt, Germany. The repository was actively used for disposal up to 1998 and contains approximately 37,000 cubic meters of waste. Its operator, the Federal Office for Radiation Protection (BfS), is currently in the process of planning for decommissioning of the repository. The underground tour included visits to various galleries and a couple of very large rooms. Of special note to the writer was the purity and clarity of the rock salt at this facility, much more so than other rock salts he has seen. The tour of the mining damage region Staßfurt included surface visits to various areas where sinkholes at the surface had formed, due to mining activities, with an explanation of the mechanisms that led to the damage, as well as a discussion and brief history of the mining activities in the region. Interestingly, one such sinkhole was now a lake in the center of a city and was being used as a recreational facility.

3. TWELFTH JOINT PROJECT III MEETING

The author attended the quarterly project meeting (workshop) of the US-German Joint Project on "Comparison of Current Constitutive Models and Simulation Procedures on the Basis of Model Calculations of the Thermo-Mechanical Behavior and Healing of Rock Salt" (hereafter Joint Project III) held at KIT-Veranstaltungszentrum Ostendorf-Haus in Karlsruhe. Alexandra Pudewills of KIT served as our host. The purpose of the meeting was to bring all of the partners up-to-date on the progress of the ongoing work since the last quarterly meeting. Following a brief welcome and an introduction to the agenda by Andreas Hampel, the status of the laboratory tests on WIPP salt was presented first. Salzer presented an overview of the recent shipments, preparations of specimens and the lab test program with rock salt from WIPP. Almost all specimens have been produced; about 50 specimens of argillaceous salt were delivered to TUC. BGR has gotten some specimens for additional creep tests at higher temperatures (100, 120, 140 °C). IfG has performed petro-physical investigations; this work demonstrates that the salt type “clean salt” from WIPP is indeed very clean. Humidity investigations of the clean salt gave values of less than 0.2 wt.-% with an average of 0.15 wt.-%. Argillaceous salt yielded values of less than 0.8 wt.-% with an average of 0.4 wt.-%. Domal salt usually has a humidity of 0.02 wt.-%. Strength tests with the clean salt have been completed. The standard strain rate was 10E-5

1/s, tests with 10E-4 1/s show a higher failure stress, tests with 10E-6 1/s a lower failure stress. All creep tests but one have been completed, one test at 60°C is still running. Herchen then presented results of TUC lab tests with older clean rock salt from WIPP (performed until 09/2013) as well as results of the first strength tests with a strain rate of 10E-5 1/s with argillaceous salt from the recent drillings at WIPP. Each test has an interposed unloading/loading phase for the determination of Young's modulus. TUC will try to complete the strength tests with argillaceous salt within the next weeks so that the data can be used for the determination of model parameter values by the partners by the next meeting.

The next series of presentations were by Pudewills, Hampel, and Gährken, and covered the back-calculations of lab tests and the IFC&HFCP in-situ tests. Both Pudewills and Hampel presented results of their back-calculations of the recent creep and strength tests of IfG, and of the healing tests of TUC. Hampel used this exercise to adjust two parameters of his CDM model to the IFC in-situ test data. The resulting set of parameter values was then used in his Dammjoch simulations.

Various presentations related to the progress on the Dammjoch (bulkhead) numerical modeling of damage and healing followed. Pudewills, Herchen, Yildirim, Günther, and Hampel presented the bulkhead results obtained with their respective models. There was also discussion on which results are to be compared among the partners and what variants of the analysis are to be completed. This Dammjoch simulation was performed only by the German partners over the past year - Sandia did not perform these simulations due to funding constraints last year. By next workshop, Hampel will compile and compare the bulkhead simulation results of the various participants.

In preparation for the start of the WIPP Rooms B & D calculations that the partners will perform, the writer was asked to provide a starting mesh for WIPP Room D to all the partners. The writer explained the structure of salt layers around Room D at WIPP and the contents of his coarse model data file that he had sent previously to the partners. The data file contains the nodes, 4 blocks of material types (clean salt, argillaceous salt, anhydrite, and polyhalite), roller boundaries on both model sides, slide conditions on clay seams, and the loads on the top and bottom model surfaces. Only one material block edge at the upper right model corner is fixed. The rest of the top surface and the complete bottom surface have an applied stress condition in order to account for the correct uplift of the floor and downward movement of the ceiling of Room D. The length unit in the data file is meters. The material properties of the various material blocks and clay seams shall be used as given in the IJRMMS paper by D. E. Munson (Munson 1997). The writer will compile a table of these properties for the partners.

The next Joint Project III quarterly meeting was scheduled and is to be held May 28th-29th 2014 in Albuquerque, NM, with Sandia hosting. A tour of WIPP was requested by Salzer, given that he has never visited and he has an interest in viewing the area from which the WIPP salt samples that IfG is testing were obtained. Others may join him on this tour which is being planned adjacent to the Joint Project III meeting dates. Unfortunately, a fire and radiological release at WIPP closed it in February.

4. WORK ON PRELIMINARY JOINT PROJECT III WIPP BENCHMARKING PROBLEMS DEFINITION

In preparation for the WIPP Room B and D benchmarking exercise that is to be undertaken by all partners of the US-German Joint Project III, the author performed additional preliminary analyses that will help guide the final specification and description of the benchmark problems. To put the current efforts in the proper context it is necessary to provide some background to earlier analytical 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). These 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 as the “legacy calculations.”

Introduction – 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 (compared to today) and limited memory (compared to today) were the norm for the thermo-mechanical analytical 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 an answer. If the refinement of the model was too fine, it would either not fit into random access memory (RAM) and/or it would take an incredibly long time to run. Refinement of a model has always been an important consideration when performing a numerical simulation and it was well-known 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., days, rather than 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 creep thermo-mechanical problems of that day.

30 Years of Advancements – The ensuing thirty years since those early days have led to significant advancements and these have yielded efficient frameworks and enabling tools/infrastructure to produce a new generation of high-fidelity simulation tools, incorporating advances in both hardware (computers) and software (algorithms and computer programs). In 2014, parallel and/or massively parallel computers (clusters) 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 servers 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 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 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.

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 code suite for this class of problems. The rooms are identical and are located at the same depth within the stratigraphy. Hence, the only difference between them is that Room D is an isothermal room, while Room B is a heated room. Up to now, work has focused on trying to duplicate the results from the legacy calculations of Munson and co-workers (Argüello and Rath 2012, 2013). Note that the work reported in the Munson (1997) article 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 through the mid-1990s (Munson, et al. 1989, Munson et al. 1990b, Munson and DeVries 1991, and Callahan and DeVries 1992) and culminated in the Munson (1997) article. In trying to duplicate the results of the legacy calculations on WIPP Room 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 Room D and B legacy calculations of Munson and co-workers has been an issue because the size of the model(s) used and/or a figure showing the mesh that was used are absent in the documentation of the various results.

However, the work of Morgan and Stone (1985) does provide such information on model size. So, in lieu of no problem-size information from the legacy calculations documentation, a mesh similar to that of Morgan and Stone (1985) was used for duplicating the legacy WIPP Room D calculations. This model configuration is shown in Figure 1, and the mesh, shown in Figure 2, is representative of the refinement used 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 consisted 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 three-dimensional). It also contained four element blocks that represent the four materials: clean salt, argillaceous salt, anhydrite, and polyhalite. The nine clay seams nearest the room were included in this model as infinitely thin sliding surfaces and 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 a coefficient of friction. The coefficient of friction was taken as 0.2 for all sliding surfaces in the calculations.

Tractions of 13.57 MPa at the top (that account for the weight of the overburden) and 15.97 MPa at the bottom of the model (that include the weight of the material in the idealized configuration minus the room) were included. The boundary conditions in the model were such that there was no horizontal displacement permitted on the sides and the upper-most material layer's right edge was prevented from displacing in either the vertical or horizontal directions (to preclude rigid-body movement).

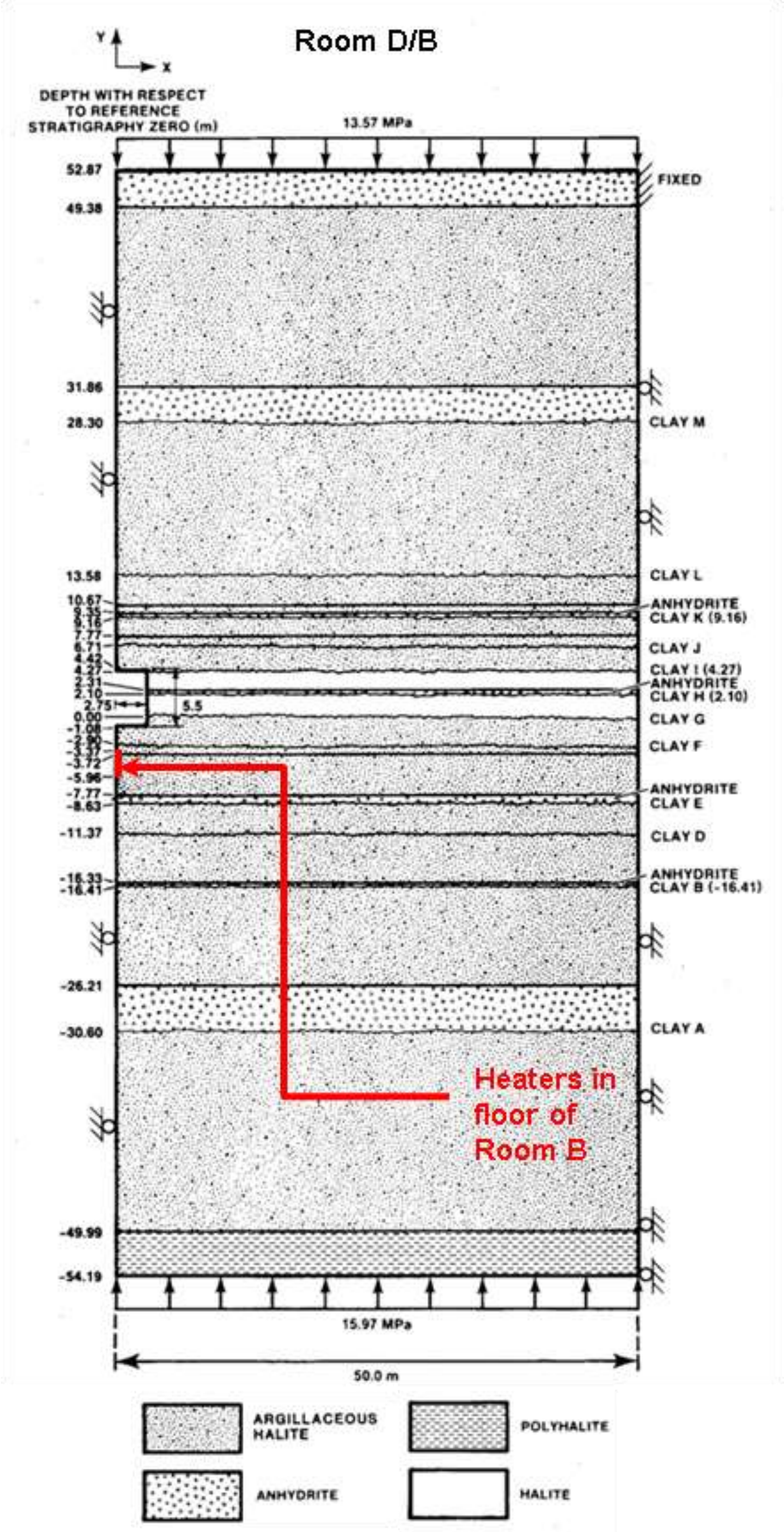

Figure 1. WIPP Rooms D/B Model Configuration – Idealization and Stratigraphy

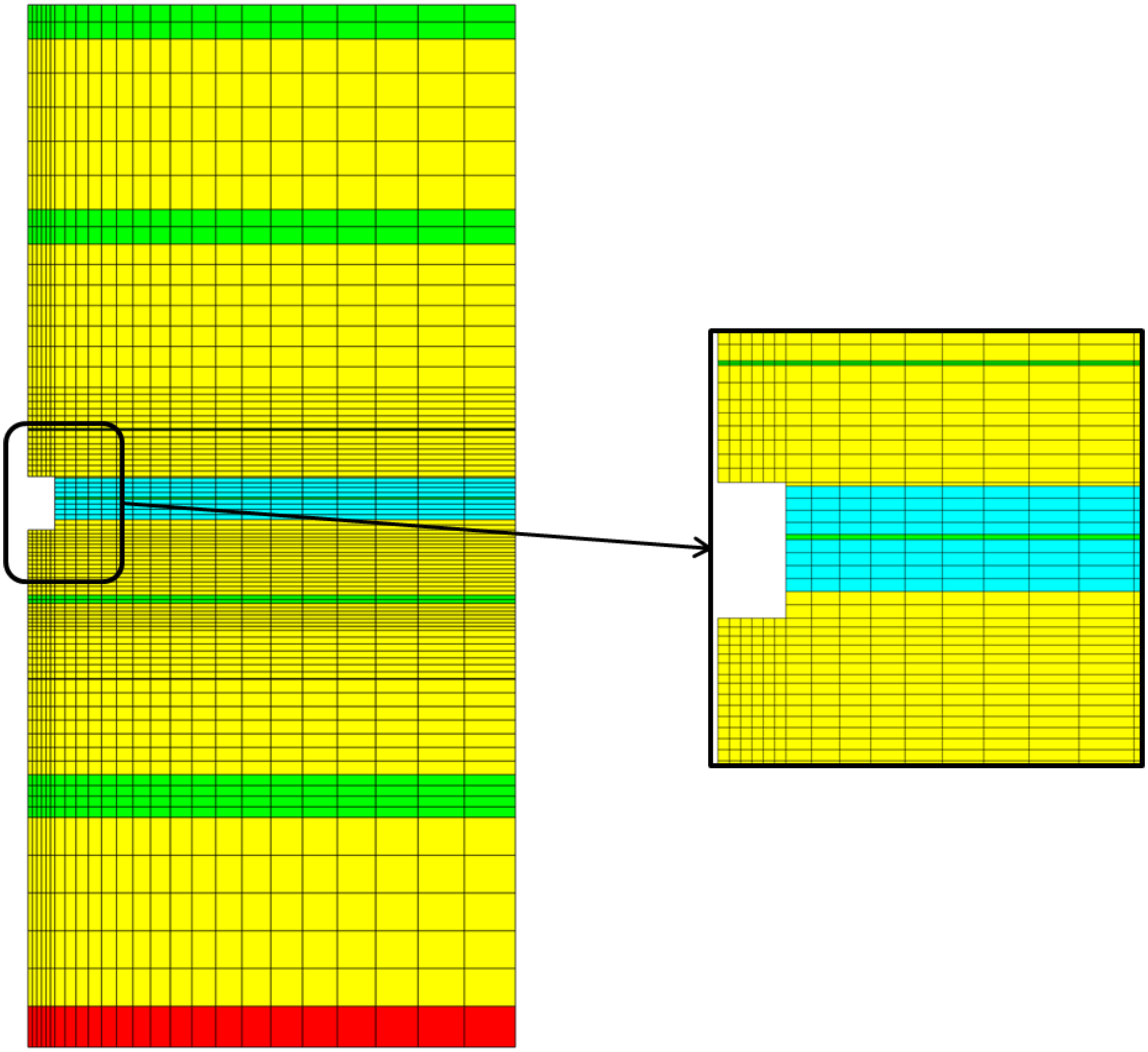

Figure 2. WIPP Rooms D/B Mesh – Consistent with Typical One Used in Mid-1980s

By current standards, this mesh is relatively coarse. However, the original goal of the current effort 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 was used. The salt was modeled with the M-D Creep Model. Because the M-D model is well-described elsewhere (e.g., Munson et al. 1989a, Munson 1997), it will not be repeated here. However, the M-D Creep Model properties for clean and argillaceous salt that were used in these calculations are given in Table 1.

Table 1. M-D Creep Model Parameter for Clean and Argillaceous Salt (differences from Clean Salt in Blue)

	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		3.034×10^{-2} (4.289×10^{-2})
	Activation energies	Q_1	cal/mole	25,000
		Q_2	cal/mole	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} (1.783×10^{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

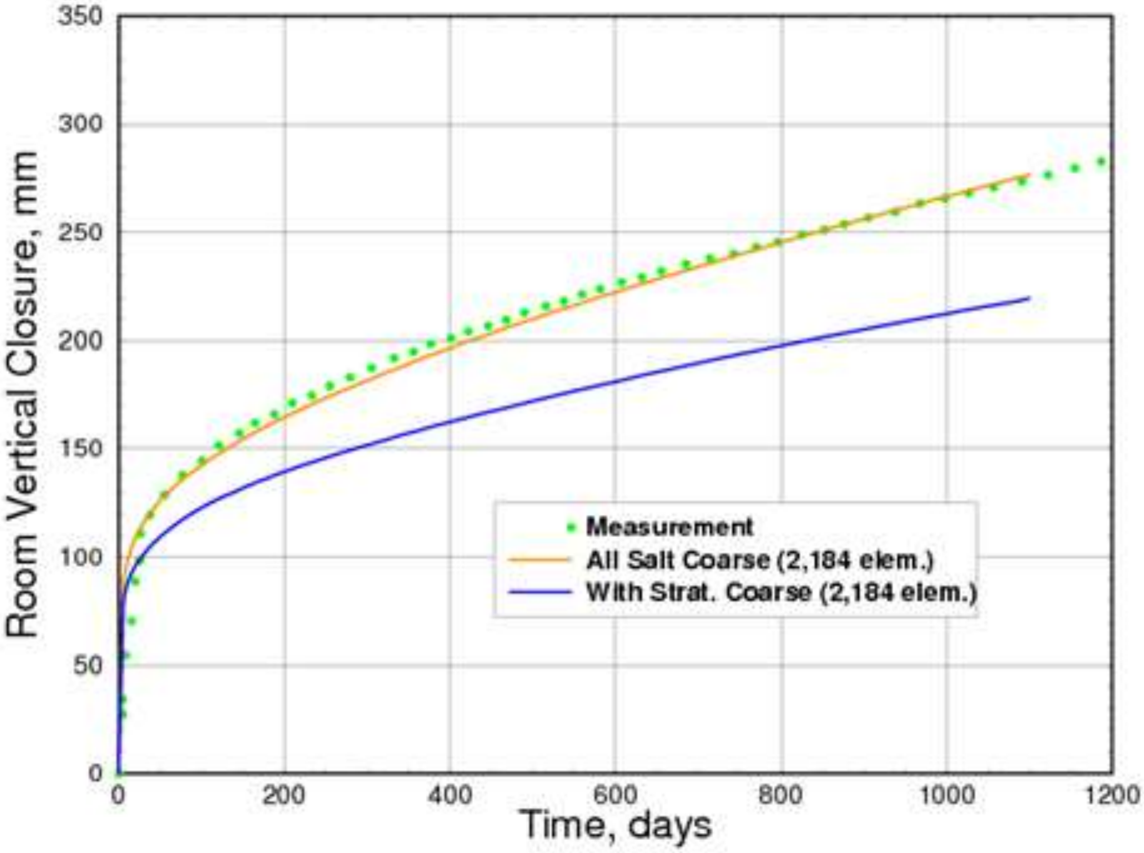

Figure 3. Room D Vertical Closure Results with "Original" Mesh Compared to Measurements

By all-salt, it is meant that the anhydrite and polyhalite were treated as if they were actually clean salt. 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 simulate 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 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).

The full stratigraphy results used distinctly different properties from salt for the anhydrite and polyhalite. They also used a different constitutive model for the representation of their behavior.

The anhydrite and polyhalite were modeled with an elastic, perfectly-plastic Drucker-Prager criterion: $F = \sqrt{J_2} + aI_1 - C$, where $I_1 = \sigma_{kk}$; $J_2 = S_{ij}S_{ji}$; and a & C are material constants. The parameters for the two materials are shown in Table 2. As seen in Figure 3, the computed vertical closure results with the full-stratigraphy for Room D lie below the measured values throughout the simulation time.

Table 2. Drucker-Prager Material Parameters

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

The latest work in the current effort focusses on developing a benchmark problem definition for the US-German Joint Project III. 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. 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. 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 still lies below the measured value, but closer than what was seen with the original mesh. 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. Consequently, the all-salt stratigraphy case and the full stratigraphy case are bracketing the measured vertical closure of the room. So it appears that in the legacy calculations, the MD parameters (as well as other features in the model, e.g., coefficient of friction) were calibrated to match the tests using a relatively coarse mesh that was quite reasonable at the time. This remains an open question that we hope to address under the US-German Joint Project III as we exercise the two WIPP rooms under the benchmarking exercise. It further implies that a common refinement of the room model among the partners may be needed to be able to make appropriate comparisons between the results of the various partners participating in the benchmark.

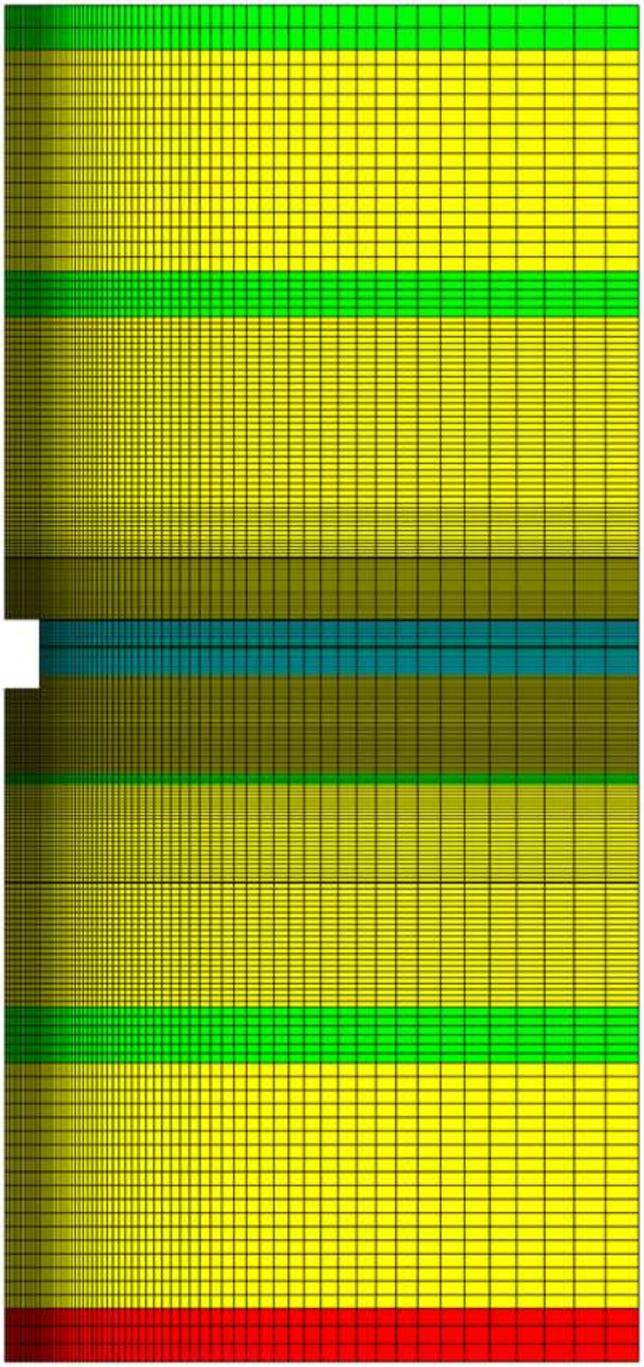

Figure 4. Refined WIPP Room D Mesh with ~8X Elements of Original

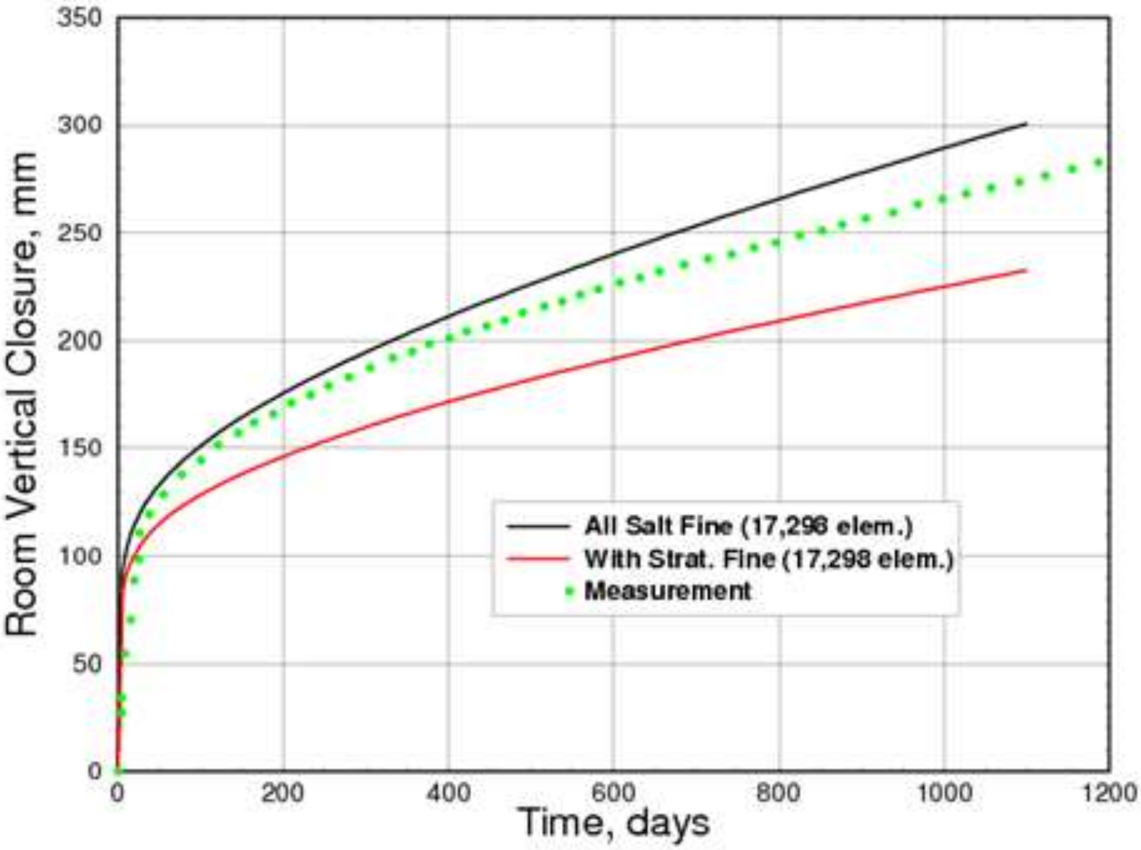

Figure 5. Room D Vertical Closure Results with "Refined" Mesh Compared to Measurements

5. PARTICIPATION AND PRESENTATIONS AT VARIOUS MEETINGS

The author participated and made various presentations related to the international benchmarking activities. First was the March 19, 2014 meeting of the US Nuclear Waste Technical Review Board (NWTRB) in which the author was asked to present on a "Coupled Model for Thermal-Hydrological-Mechanical (THM) Processes in a High-Level Radioactive Waste (HLW) Repository in Salt" (SAND2014-1349P). This presentation discussed the ongoing efforts by Sandia to develop a capability to simulate coupled THM processes in a HLW repository. In it, the effort at adapting the SIERRA Mechanics code suite for geologic repository applications was described. In addition, it also included a description of the current collaboration between DOE and German investigators to study the thermo-mechanical behavior and sealing/healing of salt – examples of comparisons between field data from the Asse salt mine and simulation results were included. It included, as well, a description of a scoping thermo-mechanical simulation with SIERRA Mechanics to evaluate room closure in a generic HLW salt repository. NWTRB response to this effort was very positive and issued the following comment on the work after subsequent to the meeting: "The Board commends DOE for the significant progress that has been made in developing a state-of-the-art thermal-hydrological-mechanical model for repository applications and urges the group to continue its efforts in model improvement, including incorporation of thin clay beds that can have significant impact on mechanical performance, and, most importantly, in model validation using field data available from U.S. and international sites."

The author also participated with an article (Argüello 2014) and presented at the 48th US Rock Mechanics / Geomechanics Symposium in early June on the "Potential Use of Geologic Rock Salt for Fuel Cycle Sustainability – a Computational Modeling Perspective" (SAND2014-4335C). The various components that make up a computational modeling capability to address the thermo-mechanical behavior of rock salt over a wide range of time and space were first presented. The solver technology that is required to address the large deformation, highly nonlinear, nature of the repository was also addressed, in general. Included were the features of a valid constitutive model needed to capture the important phenomena of rock salt creep deformation over repository performance ranges. Also in this discussion were the typical issues of importance in computational models, i.e., discretization, stability, accuracy, etc. Confidence in computational models is attained by grounding the models on sound physical principles, first, and then using acceptable mathematical and numerical methods to represent the behavior. They are then validated through a systematic process that includes exercising the model to solve a basic problem (one with a known solution, if possible); comparing model response against behavior of natural known phenomena; conducting laboratory, bench-scale, and field tests to evaluate the performance of the model's predictions; and conducting in-situ tests to compare predictive results of the model with actual underground data. In this vein, several example rock salt calculations were presented to demonstrate the applicability and validity of the modeling capability described in the presentation to repository-scale problems. These varied from simple problems designed to test elementary creep response behavior to the more complex that dealt with addressing specific aspects of repository room behavior. This latter set of problems included the Sandia benchmark results for the IFC and HFCP problems of the US-German Joint Project III.

A third meeting that the author participated in was the June 2014 UFD Working Group Meeting Las Vegas. Specifically he reported on the status of the international collaborations with the Germans under the US-German Joint Project III at the breakout session on International Disposal Research. This session discussed the status of ongoing work and new opportunities for international disposal R&D. Participants were asked to also take stock of the international collaborations activities conducted so far, elaborate as to how they have benefitted the UFD campaign, and discussed what goes well in the international work and what does not, including whether any changes in the scope or direction were intended in the future. The author provided a brief verbal overview report outlining the work to date on the salt benchmark modeling activities with the Germans.

6. THIRTEENTH JOINT PROJECT III MEETING

The author participated the latest (13th) quarterly project meeting of the US-German Joint Project on "Comparison of Current Constitutive Models and Simulation Procedures on the Basis of Model Calculations of the Thermo-Mechanical Behavior and Healing of Rock Salt" (Joint Project III) held at Sandia National Laboratories' Innovation Parkway Office Center (IPOC) in Albuquerque, NM. Frank Hansen and the author served as co-hosts of the meeting. Because this meeting was in the Albuquerque (typically held in Germany) this time, it facilitated additional attendees from the US at this meeting from both Sandia and RESPEC.

This meeting focused on the comparison of results of the Dammjoch bulkhead simulations and some initial work on the WIPP benchmark study that looks at temperature influence on deformation. With regard to the latter, focus was on the performance and evaluation of an extensive laboratory test program with WIPP salt that the Germans have been conducting and the re-calculation of laboratory tests to determine parameter values for WIPP salt.

The purpose of the meeting was to bring all of the partners up-to-date on the progress of the ongoing work since the last quarterly meeting. Following a brief welcome and an introduction to the agenda by Andreas Hampel, the status of the laboratory tests on WIPP salt was presented first. Klaus Salzer of IfG talked about the shipment of cores, the preparation of the specimens, and the laboratory testing program with rock salt from WIPP being carried out at IfG. Approximately 150 cylindrical samples have been or will be prepared at IfG from the larger clean and argillaceous salt cylinders shipped from WIPP. Petro-physical characterization was performed on the samples and the clean salt was found to be very pure salt with low amounts of impurities. The initial porosity of the samples was also low, indicating that the salt is undisturbed. In short Salzer stated that this was excellent material. The water content (weight percent) of the clean salt (0.15) was found to be less than that for the argillaceous salt (0.4), and is therefore generally higher than for domal rock salt. Salzer then described the triaxial strength testing of the salt specimens and showed a figure demonstrating the transition of the material from brittle to semi-brittle to ductile with increasing confining stress from 0.2 MPa to 20.0 MPa, when tested at 25 C. Strength testing of the salt at 60 and 100 C was also performed. The strength was found to be slightly lower than for Asse salt, but the dilatancy boundary was found to be similar. Salzer then described the multi-stage creep testing performed at IfG. This is done with a new IfG creep test rig that uses stress control to overcome several short-comings of earlier test machines. Creep testing on clean salt was performed on samples at 24, 60, and 80 C, with stress changes of 12, 18, and 8 MPa. The results show slightly higher creep rates compared to Asse salt. Additional standard tests are still ongoing and will require additional time to complete. Furthermore there are special healing tests still to be carried out by TUC.

Kai Herchen, from TUC, gave the next presentation on the results of the TUC lab tests with argillaceous salt from WIPP. As of May 2014, twenty seven strength tests have been carried out at TUC at temperatures of 27, 60, and 100 C. The confining stress on these tests has varied from 1 to 20 MPa. In addition, they have carried out eight creep tests. So far their creep tests on the argillaceous salt have been carried out at temperatures of 27 and 60 C, although they have plans to test also at 80 C. Mr. Herchen then described their process for the determination of the failure strength envelope from the strength tests and the determination of the creep rate from the creep tests. He also described the TUC lab procedure and methods to determine dilatancy. In the process of the presentation, he also gave a brief overview of the TUC test equipment and the climate chamber that is used for some of the tests.

The next presentation was given by Andreas Gährken, of TUBS, on the comparison of laboratory test results: clean salt – argillaceous salt – Asse-Speisesalz. First off, there was a brief summary presented of all the strength tests and creep tests conducted under similar conditions for the three salts: Asse-Speisesalz, WIPP Clean Salt, and WIPP Argillaceous Salt. For example, strength tests have been conducted on all three salts at a confining stress of 2 MPa and nominally at the same temperature (26.85, 25, and 27 C for Asse-Speisesalz, WIPP Clean Salt, and WIPP

Argillaceous Salt, respectively). Likewise, for the creep tests, where for example Asse-Speisesalz and WIPP Clean Salt have been tested at the same levels of stress difference, but the former at 59.85 C and the latter at 60 C. When summarized, the overall results showed that all three respond similarly in terms of strength. For example, if the salts are compared at a nominal temperature of 27 C when tested at a strain rate of 1.0E-5 per second, the failure boundary is slightly higher for Asse-Speisesalz compared to the WIPP Clean Salt and a bit lower for the WIPP Argillaceous Salt. Under these conditions, the dilatancy boundary was shown to again be similar with that of the Asse-Speisesalz and the WIPP Clean Salt being roughly equal and the WIPP Argillaceous Salt being a bit lower. There was no perceptible difference in the residual strength of the salts. For the creep tests, it was generally shown that the WIPP Clean Salt creeps at a slightly higher rate than Asse-Speisesalz.

The next presentation was given by Hampel on a re-evaluation of Sandia’s lab test data from the 90s and comparison of the results with those from the recent lab test series of IfG and TUC. The focus of this re-evaluation was on steady-state creep. By “old” Sandia tests he means the set of tests that were performed on rock salt from the WIPP from 1979 to 1992 – he showed a table containing 89 tests. He compared these to what he refers to as the “old” BGR test on Speisesalz performed from 1990 to 1999, as well as what he refers to as the new IfG tests on Speisesalz (same layer, different locations) run recently in the 2011 to 2012 timeframe. He also makes reference to the new IfG tests on WIPP clean salt which have also been run recently in the 2013 to 2014 timeframe. In his re-evaluation and for determination of the steady-state creep rate, Hampel made use of five types of graphs: temperature versus time; stress difference versus time; strain versus time; strain rate versus time; and strain rate versus strain. The method that he used for re-evaluation of the creep tests was to check if: (1) boundary conditions (Temperature, stress-difference, and confining stress) are constant; (2) stress versus time curve has a good quality (smooth, monotone); (3) stress state is below the dilatancy boundary (there is no damage influence); (4) a sufficient total deformation per test stage is reached; and (5) “true” steady-state creep is reached. Hampel provided several examples of the various graphs as he demonstrated the method that he used. For example, in one case, he showed a test in which a constant stress difference is apparent, but another in which there were small fluctuations, but which he considered as being insignificant for his purposes, as opposed to a third case in which there were both fluctuations and drift apparent in the data, potentially rendering the data invalid. So for example in this latter case, the steady-state creep rate before the onset of drift is possibly determinable but before that can be determined, one must check the other criteria. He also showed additional examples, including one in which the damage influence was not clearly visible at the creep curve level but revealed itself only when the stress state was checked, thereby rendering that curve invalid for determination of steady-state creep. With regard to the question of the attainment of sufficient total deformation per test stage, Hampel showed an example where insufficient total deformation can be misleading. Another point that was made in this presentation was that the higher the stress-difference, the more deformation that is necessary to reach the steady-state micro-structure and steady-state creep. Finally, in evaluating the creep tests, Hampel developed a “quality ranking” for the determination of steady-state creep rates ranging from a numerical value of five to one, with five meaning that steady-state creep is reliably reached (i.e., most certain results) to one where it is not possible to be determined. Of the various “old” Sandia tests, twenty-one of them in the lower temperature range (21–32 C) were found to be of quality ranking 4 or higher. Likewise ten in the temperature range of 100–107 C, ten of the “old” tests were found to be of quality ranking 4 or higher, and in the temperature range 209–212 C, seven of the “old” tests were found to be of quality ranking 4 or higher. In light of he re-evaluation, Hampel offered the following conclusions:

- Steady-state creep rates from the “old” Sandia tests and new IfG tests with “clean salt” from WIPP match;
- In the temperature range from, 20–110 °C, the “Clean salt” from WIPP creeps faster (factor of 2–10) than Asse-Speisesalz;
- At a temperature of around 200 °C, the rates coincide, at least at stress differences greater than or equal to 5 MPa; and
- For both salt types, the stress exponent n ~ 3–5 at smaller stress differences and temperatures, and n ~ 7 at higher stress differences.

Hampel’s presentation was followed by several Sandia presentations that were essentially previews of presentations that were presented the following week at the 48th US Rock Mechanics / Geomechanics Symposium in Minnesota. The presentations by Broome and Bauer covered the various capabilities to perform lab tests and thermo-physical investigations and results of recent investigations of WIPP crushed salt consolidation at high temperature. Bauer presented on “Experimental Determinations of Thermo-physical Properties of Reconsolidated Crushed Salt” and Broome presented on “Reconsolidation of Crushed Salt to 250°C under Hydrostatic and Shear Stress Conditions.” Hansen presented on the “Micromechanics of Isochoric Salt Deformation.” In addition, Shoemaker gave the German partners a briefing on the status of WIPP as of May 2014, following the earlier radiological release accident there. Prior to the accident, it had been the request of several of the German participants, some who had never visited WIPP before, to tour the underground at WIPP, similar to what we had done two years ago. Unfortunately this was not possible and instead a tour of the neighboring Mosaic Potash Mine was undertaken by those participants.

Following the Sandia presentations, Hampel again led the discussion of the comparison of results of the bulkhead (Dammjoch) simulations that were performed by the various German partners. The bulkhead is located in a drift at the 700 m depth in the Asse Mine. The drift, with a maximum height of 2.75 m and a maximum width of 3.8 m was excavated in 1911. In 1914 a 25 m long section of the drift was lined with a cast-steel tube that was 2.30 m in diameter with a wall thickness of 10 cm. The residual gap between the drift wall and the tube was filled with concrete. A common model of the bulkhead, prepared by Günther was used by each partner for this benchmarking problem. Two simulations were performed. The first simulation was of an open drift to compute its free convergence response during 88 years. A second simulation was performed in which the response was computed for an open drift for 3 years. This was then followed by the addition of the bulkhead (cast-steel tube and concrete) and computing the response of the drift with the bulkhead installed for another 85 years. There were unique parameters for the cast-steel tube (assumed elastic), the concrete (assumed elastic), and the rock salt used by each partner. There were also unique boundary/initial conditions used by each partner for the state of the configuration, namely a temperature of 35 °C and an initial stress of 15 MPa at the 700 m depth. In terms of quantities for evaluation – displacements, principal stress components, equivalent stress, total strain, and volumetric strains were tracked by each partner at eight history locations – with output traces horizontally into the salt; diagonally down (45 degrees), or vertically down. The various location are as follows: H1 located at center of drift ceiling; H2 located at drift wall at half height; H3 located at drift wall, 45° down; H4 located at center of drift floor; H6 located at 15 cm below drift floor; and H8 located at 17 cm behind drift wall.

The remainder of the presentation, and in fact the bulk of the remainder of the day, was a detailed look and assessment of the results collected from each of the partners on: (1) the open drift histories; (2) the histories with the bulkhead; (3) the horizontal traces; (4) the vertical traces and (5) the diagonal traces. For the first simulation with the open drift, only the last three items were requested. For the second simulation with the bulkhead, the results in which healing was assumed were compared to the results with no healing assumed. One general conclusion that the author drew from this very detailed look at the various approaches used for modeling healing by the different German partners is that there is no general consensus yet on an approach to model healing once the simulation goes from modeling a laboratory test to modeling a complex underground problem such as this bulkhead. While each of the different German groups has a different approach for modeling healing that works on laboratory tests with well-prescribed boundary conditions, the different approaches appear to yield very disparate results on true underground configurations where the conditions of loading are multi-axial and more complex. In short, it appears that the healing component of these models is still relatively immature as of May 2014.

There were several items on the agenda that were not covered because of the longer-than-expected discussions on the bulkhead simulations. Among these was a look at the various partners' re-calculation of the various WIPP salt laboratory tests with a unique set of parameters determined from all tests. In addition, a look at the partners' preliminary simulations of WIPP Room D was not possible, although it appears that not all of the partners are yet engaged on the Room D simulation as of May 2014.

The week of October 13–17th was tentatively scheduled for next JP III workshop in the area of Mainz, Germany.

7. 5th US-GERMAN WORKSHOP ON SALT REPOSITORY RESEARCH, DESIGN, AND OPERATIONS

This meeting is a more general US-German workshop on Salt Repositories (as opposed to only constitutive modeling and simulation procedures) and the writer presented the status of the US contribution of the work carried-out to date on the US-German Joint Project III to a broader audience. Sessions on Repository Operational Safety; Retrievability and Repository Design; TM-Behavior of Salt; Plugging and Sealing; Safety Case and Performance Assessment; Special Topics; and Specially Scheduled Breakout Sessions were included in the agenda for the workshop. The presentation entitled: "Modeling WIPP Rooms D and B'" (SAND2014-16886PE) was presented by the author in the "TM-Behavior of Salt" session. He also participated in the discussions/interactions related to the more general issue of applicability of the results from the US-German Joint Project III to a potential repository sited in rock salt and addressed questions related to the interfacing and coupling of the thermo-mechanical effects with other physics of importance in a repository setting (i.e., hydrological, chemical, etc. effects).

8. SUMMARY

Various activities continued in the area of international benchmark calculations of field experiments during FY14. The work is being carried out under the auspices of a US-German Joint Project to look at current constitutive models and simulation procedures for the thermo-mechanical behavior and healing of rock salt.

In addition to the Asse Mine benchmark problems that have been performed to date, that are located in domal salt, Joint Project III was recently extended (with funding on the German side) to include two additional problems in bedded salt: WIPP Rooms D and B. In preparation for their calculational efforts, the German scientists requested and received WIPP salt core for the purpose of laboratory testing to carry out special tests required for their constitutive models.

In supporting the above, the writer has made technical presentations and interacted with the Germans scientific community in various venues as described herein. Much of the overall effort has been in sharing his experiences on some preliminary work that has been done recently in re-visiting the WIPP Rooms D and B in-situ experiments. In addition, newer efforts aimed at defining the benchmark problems have led to refining the computational mesh over that used previously, to be more in line with current practice/standards. In doing so, it was found that the computed vertical closure response of Room D was greater than previously computed with the original (coarse) mesh. This implies that perhaps, in the legacy model of the rooms and calculations, the MD parameters (and other features of the model) were calibrated to match the tests using a relatively coarse mesh that was acceptable at the time, but that now appears too coarse. This remains an open question that we hope to answer under Joint Project III. Furthermore, this implies that a common refinement of the room among the partners may be needed to make appropriate comparisons between the results of the various partners participating in the benchmark exercise.

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