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Summary of FY15 Results of Benchmark Modeling Activities

Fuel Cycle Research & Development

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QA program which meets the requirements of
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SUMMARY

Sandia is participating in 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 required to address this 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 FY15 in support of this international U.S.-German benchmark initiative.

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

ANSYS	Engineering Simulation Software
BMWi	German Federal Ministry for Economic Affairs and Energy
CDM	Composite Dilatancy Model
DOE	Department of Energy
EDZ	Excavation Damaged Zone
FLAC	Fast Lagrangian Analysis Code
FCR&D	Fuel Cycle Research & Development
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
KIT	Karlsruher Institut für Technologie
LUH	Leibniz Universität Hannover
M-D	Multi-mechanism Deformation
NE	Office of Nuclear Energy
POC	Point-of-Contact
SaltMech8	International Conference on the Mechanical Behavior of Salt VIII
SOA	State-of-the-Art
TSI	Thermal/Structural Interactions
TUBS	Technische Universität Braunschweig
TUC	Technische Universität Clausthal
U.S.	United States
WIPP	Waste Isolation Pilot Plant

RESULTS FROM THE U.S.-GERMAN BENCHMARK INITIATIVE FOR FY15

1. INTRODUCTION

This report serves to summarize and document work on the various activities related to the international (U.S.-German) benchmark calculations of field experiments undertaken in FY15. The activities include:

(1) Participation in and presentation in support of the Fifteenth Joint Project III meeting held at TUC in Clausthal-Zellerfeld, Germany;

(2) Participation in and presentation in support of the Sixteenth Joint Project III meeting at IfG, Leipzig, Germany;

(3) Additional calculations on the WIPP Mining Development (Room D) with mesh refinement to assist preliminary U.S.-German Joint Project III WIPP benchmarking problems definition;

(4) Participation and presentations at the Eighth Conference on the Mechanical Behavior of Salt (SaltMech 8) at the South Dakota School of Mines & Technology in Rapid City, SD; and

(5) Participation in the Eighteenth Joint Project III meeting at South Dakota School of Mines & Technology in Rapid City, SD.

An overarching effort, under these activities, has been to influence the international benchmarking work being conducted under the U.S.-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, 1990) in the early 1980s. This has resulted in the successful inclusion 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 domal, or non-bedded, 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. FIFTEENTH JOINT PROJECT III MEETING

The author attended the 15th quarterly project meeting (workshop) of the U.S.-German Joint Project on “Comparison of 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), a continuing U.S.-German collaboration investigating the behavior of Rock Salt for use as a geologic medium for a nuclear waste repository. The author made contact with Savas Yildirim of LUH in Hannover on Tuesday, June 28th 2014, to finalize logistics for travel to Clausthal-Zellerfeld, as the LUH (IUB) group from Hannover was providing transportation for the author to the meeting at TUC in Clausthal-Zellerfeld. Kai Herchen and Prof. K-H Lux acted as hosts to the overall group at TUC. This technical project meeting consisted of an update by the various participants of the work performed on the project since the last meeting. The first topic covered was the completion of back-calculations of the laboratory tests with Asse-Speisesalz by the various partners; the laboratory tests modeled included healing, cyclic, and relaxation tests, with one unique set of parameter values that are also valid for creep and strength tests. Hampel also presented a comparison of stress and temperature dependencies of steady-state creep rates (T= 26, 60, 90 °C & deviatoric stress = 0 … 30 MPa) calculated by every partner with his unique set of parameter values. Hampel then briefly reviewed the submitted results of the various partners for the three in-situ test simulations (IFC, HFCP, and Dammjoch). In general, there was reasonable agreement between laboratory tests and simulations of those tests. Next, and in preparation for the WIPP Room D & B in-situ test simulations that are being performed by all partners, each partner presented his results of the back-calculation of all laboratory tests with clean salt and argillaceous salt from WIPP. Once again, in general, there was reasonable agreement between the laboratory tests and the simulations of the tests. Up next was a preliminary look at the various partners' results of their simulation of WIPP Room D (the isothermal room). A common model (modestly refined mesh) was created by IfG's Günther for the various German participants using FLAC as their analysis code, and this model was recommended for use by all partners. This model uses an all-salt stratigraphy, with all layers being clean WIPP salt, and uses the laboratory test parameter values discussed previously, i.e., parameter values determined with back-calculations of laboratory tests with clean salt from WIPP. This current model does not contain any of the clay seams (sliding surfaces) that the final model should contain. It appears from the presentations that even for this relatively straight-forward calculation for the U.S., some of the German partners are having technical difficulties (appear related to numerical integration of their models and stability of the solution). Only one or two of the German partners appear to have progressed sufficiently on this problem to make preliminary comparisons to the in-situ data.

The next topic was a review of what had been covered and learned at the 5th U.S.-German Workshop on Salt Repository Research, Design, and Operation held in Santa Fe, NM from September 7-11, 2014. Some of the partners of Joint Project III participated in the Santa Fe meeting and provided updates on the work being carried out under this Joint Project III. Among the items of discussion at the 5th U.S.-German Workshop was a discussion of future potential work between the U.S. and Germany. Part of that discussion was potential work for a succeeding "Joint Project IV." Because of what has been learned from Joint Project III, there was much discussion of this topic of Joint Project III follow-on work, among the partners, with the following list of potential tasks proposed at the end of the discussion:

- Investigation and further development of the modeling of damage reduction / healing
- Treatment of tensile stresses in model calculations
- Investigation and modeling of inhomogeneities (e.g. contact surfaces / interfaces)
- Investigation and modeling of the deformation at small deviatoric stresses

- Investigation and modeling of the humidity influence on deformation
- Deeper and more detailed analysis of the bandwidth of modeling results
- "Ranking" of constitutive models
- Modeling of crushed salt and of the transition to iact salt

Finally, there was discussion of when the next and subsequent Joint Project III quarterly meetings should be held. The next quarterly meeting will tentatively be held at the IfG in Leipzig, Germany on the 27-28th of January 2015. It was also suggested that the meeting after that one should be held in Rapid City, following SaltMech 8 (Saturday, May 30th 2015).

3. SIXTEENTH JOINT PROJECT III MEETING

The author attended the 16th quarterly project meeting (workshop) of the U.S.-German Joint Project on "Comparison of 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), a continuing U.S.-German collaboration investigating the behavior of Rock Salt for use as a geologic repository for nuclear waste. The meeting was held at the Institut für Gebirgsmechanik (IfG) in Leipzig, Germany. The day following his arrival in Leipzig, the author made contact with Andreas Hampel, the POC on the German-side, to finalize plans for travel to the IfG with Hampel. Wolfgang Minkley and the IfG acted as hosts to the overall group in Leipzig. Following a brief welcome and introduction, the first topic covered was the presentation, by various partners, of their results of the back-calculation of all laboratory tests performed with clean salt and argillaceous salt from WIPP. This was done using a unique set of salt-type-dependent parameter values determined by performing a parametric-fit to all of the numerous lab tests performed by TUC and IfG on each salt-type.

- Herchen led-off and also included re-analyses of lab tests with Asse salt (with improvements to their constitutive model in the damage regime). Re-analyses of the WIPP tests were next shown by Herchen. Herchen talked about the temperature effects on the WIPP salt. There is no temperature dependence in the transient-creep part of their model (but of course there must be because temperature dependence is seen in response of salt). It appears that there is additional work needed on their model to incorporate this effect.
- Next, Günther described the fit of the Minkley constitutive model to the various lab tests and the back-calculation of the tests. Use of this model appears be more of an art and depends highly on the application for which it is being used.
- Next, Pudewills described the multi-step creep tests back-calculation analysis results as well as the simulation of the triaxial strength tests on clean salt using their model. These were followed by the back-calculation analyses of tests on argillaceous salt.
- Finally, Hampel described back-calculations, using his model, of all lab tests with clean salt from WIPP and then he moved on to argillaceous salt. As a result of a re-look at the tests he has now improved the formulation of the CDM (his constitutive model) at higher differential stresses (because of improvements to his sinh function).

In a general and overall sense, there was reasonable agreement between the laboratory tests and the simulations of the tests by the various partners.

Up next was an updated look at the various partners' results of their simulations of the isothermal WIPP Room D. A common, modestly-refined, model was created by IfG's Günther for the various German participants that use FLAC as their analysis code, and this model was recommended for use by all partners. This model uses an all-salt stratigraphy, with all layers being clean WIPP salt, and uses the laboratory test parameter values determined previously, that is, the unique set of parameter values determined from all the laboratory tests with clean salt from WIPP. This current model does not contain any of the clay layers (sliding surfaces) that the final model should contain to allow capturing the correct horizontal closure of the room.

- Pudewills led-off with a discussion of KIT's Room D simulation. She went beyond what had been targeted, with results for Room D first using Asse properties, then WIPP clean salt properties, & finally, WIPP clean/argillaceous salt properties plus the rest of the stratigraphy. In the latter analysis, she also included sliding interfaces and got good agreement with Room D measurements (but it wasn't completely clear how she modeled the clay layers in ANSYS).
- Missal then described TUBS' calculations of WIPP Room D. He expressed frustration that there continue to be issues with completing the calculation (earlier problems in their room corners had led to the current re-calculation). It is not clear if the problems are with FLAC or with their material model.
- Yildirim described LUH's calculation of Room D but notes that they do not get the large primary creep seen in the data. They are now using the room model developed by Günther (not so previously). So it appears that LUH's calculation is still problematic.

For the Rapid City meeting, it was decided that two calculations should be completed: one with all clean salt & one with stratigraphy; but no sidelines. Andreas will send out the trace locations where results will be probed.

Next, there was extensive discussion on the upcoming meeting of the German partners with Dr. Wirth of BMWi (their funding agency) on a proposal for "Joint Project IV." Sandia's main interest in this follow-on work would be in the low deviatoric stress and interface portions of the proposal. There are new guidelines for BMWi funding from 2015–2018. Under these new guidelines salt is just one of three geologies to be considered along with claystone and granite - all of equal priority.

The next meeting of the group is proposed for March before the April 17th meeting with Dr. Wirth (March 24-25, 2015 will be a normal meeting in Braunschweig for German partners to prepare for meeting with Wirth). Thereafter, the group will meet next after the SaltMech8 meeting in Rapid City, SD.

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

In support of the WIPP Room B and D benchmarking exercise that is being undertaken by all partners of the U.S.-German Joint Project III, the author performed additional computational analyses that will help guide the final specification and description of the benchmark problems exercised under Joint Project III. This effort has mainly consisted of two sets of calculations. The first one aimed at understanding if we have reached a converged solution (in terms of mesh refinement) of the WIPP Room D problem, given that an ~8X refinement in mesh produced a computed vertical closure that was significantly different from that produced using the original coarse mesh (Argüello 2014; Argüello & Holland 2015). The second one aimed at trying to duplicate the original calculation that the German partners have decided to pursue – one in which all of the layers, shown in Figure 1 are treated as if they were clean WIPP salt. In addition, this calculation ignores all of the potential sliding at the clay seams and assumes that the stratigraphic unit above and below each of the clay seams is contiguous (i.e., no sliding surfaces are included in the calculation).

Mesh refinement calculations – In last FY's year-end report "Results from the U.S.-German Benchmark Initiative for FY14" (Argüello 2014), the author reported on some preliminary calculations completed on WIPP Room D. The write-up included a comparison of results from a coarse computational mesh – comparable to what appears to have been used in the legacy calculations of Munson and co-workers, which culminated in the work reported in the IJRMMS by Munson (1997) – to the results from a computational mesh that had been refined by ~8X the original coarse mesh. To put the present mesh refinement calculations in context, the earlier calculations will first be reviewed.

The model configuration for WIPP Room D is shown in Figure 1, and the original coarse mesh, shown in Figure 2, is representative of the refinement used in the timeframe of the legacy calculations. 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).

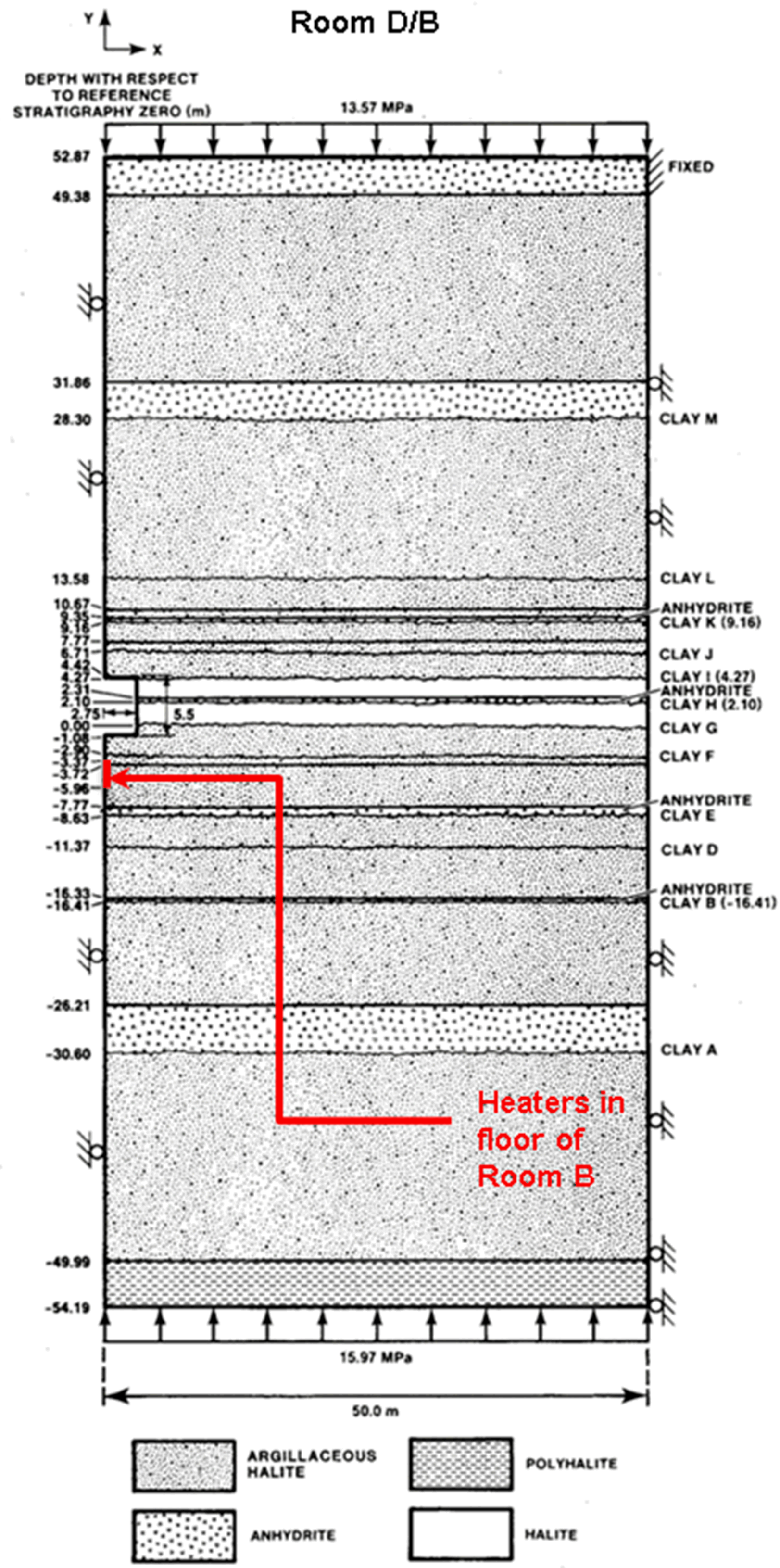

Figure 1. WIPP Rooms D/B Model Configuration – Idealization and Stratigraphy

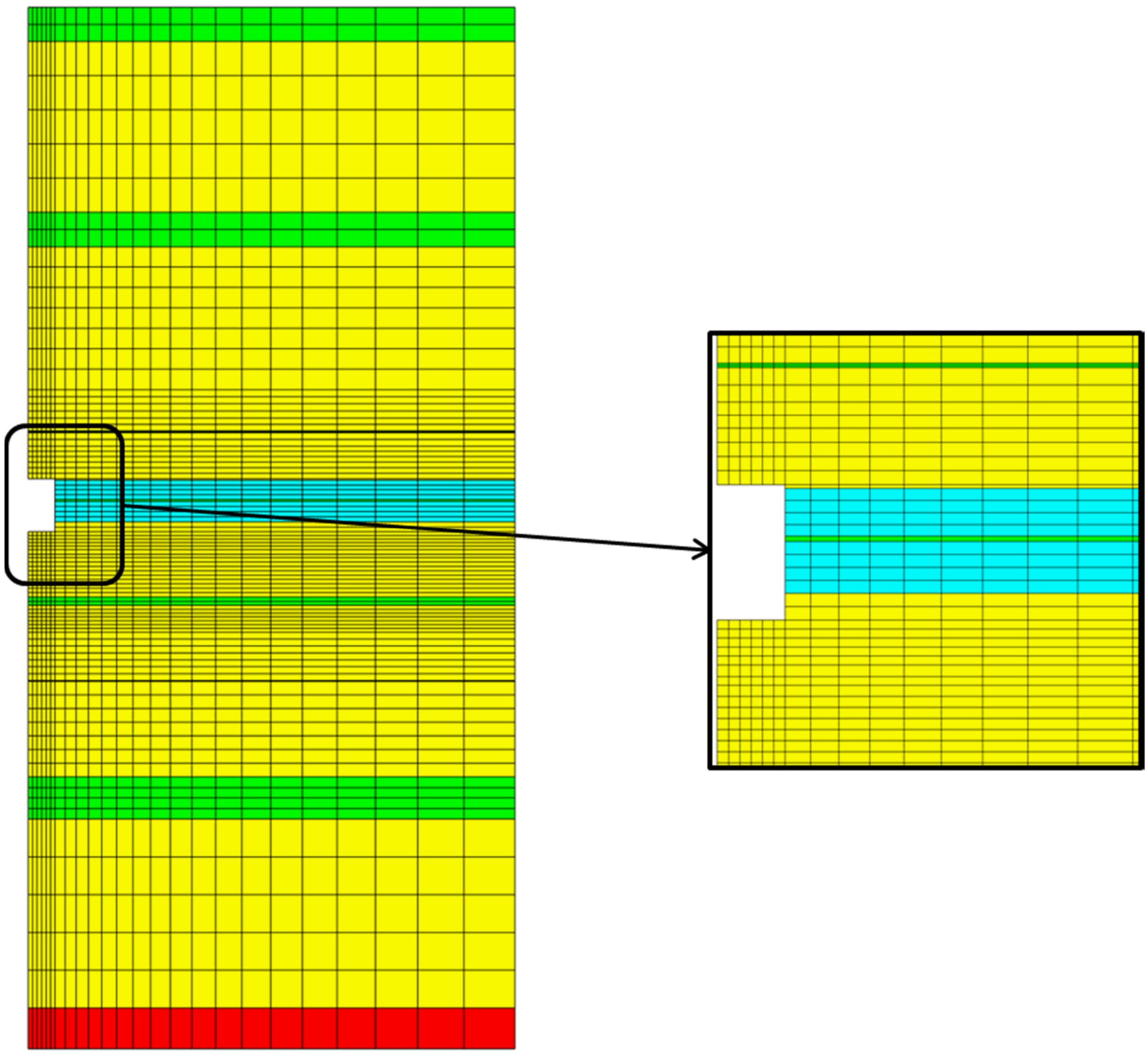

Figure 2. WIPP Rooms D/B Mesh – Consistent with Typical One Used in Mid-1980s

By current standards, this mesh is relatively coarse. 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. 1989, 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

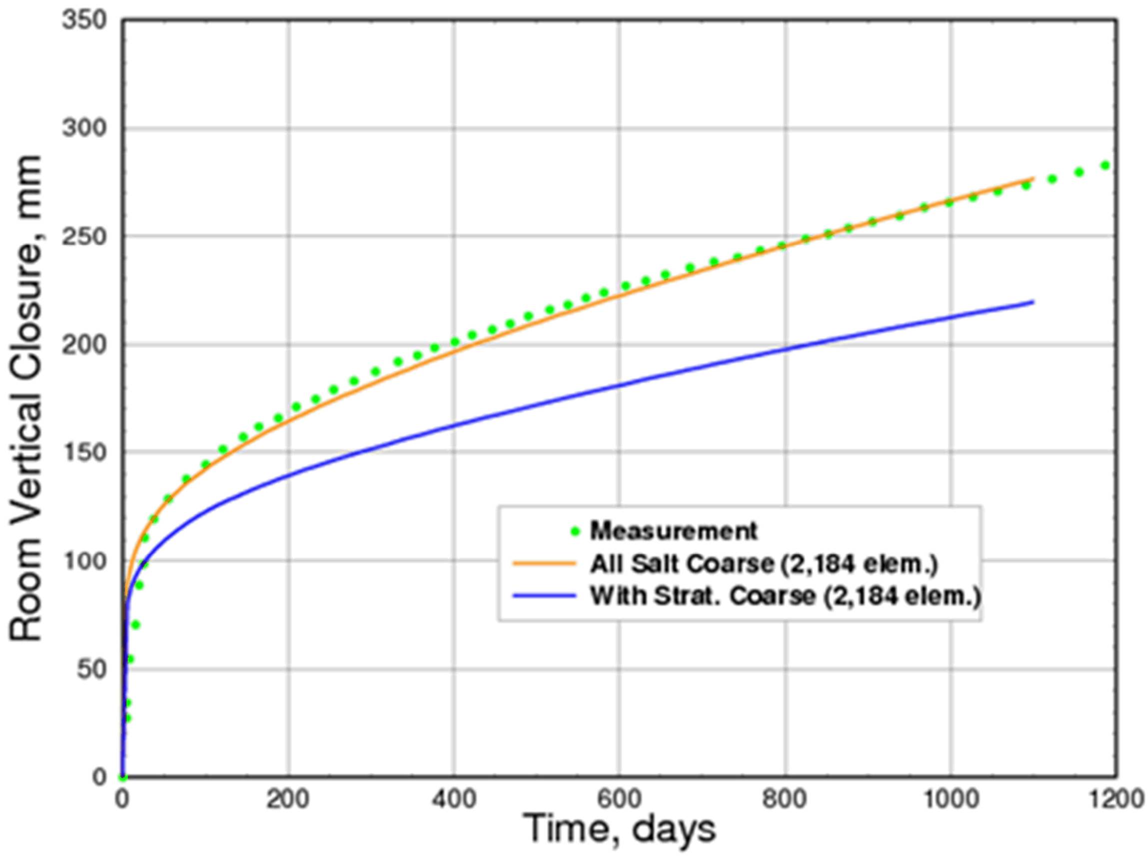

Figure 3. Room D Vertical Closure Results with "Original" Mesh Compared to Measurements

By all-salt, here 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. 1989) that looked at the response of WIPP Room D. From the Munson et al. 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. 1989).

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 and coarse mesh for Room D lie below the measured values throughout the simulation time.

Table 2. Drucker-Prager Material Parameters

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

The work in the current effort focusses on developing a benchmark problem definition for the U.S.-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.

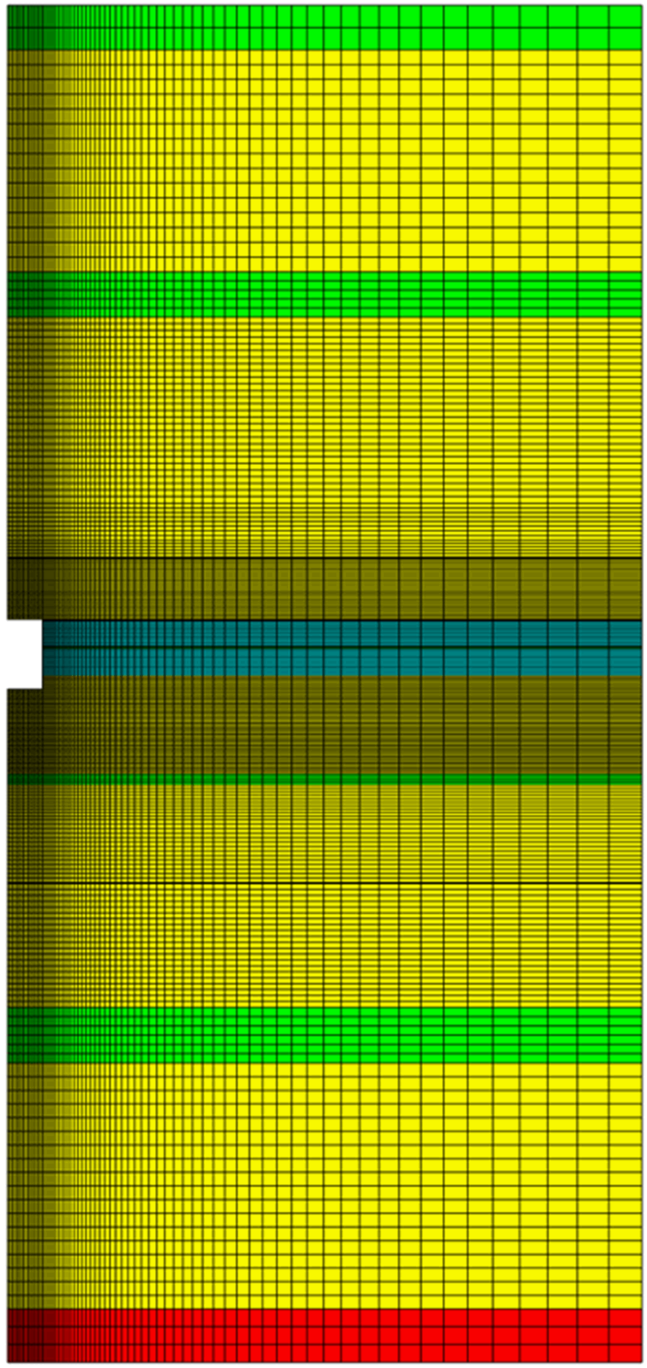

Figure 4. Refined WIPP Room D Mesh with ~8X Elements of Original

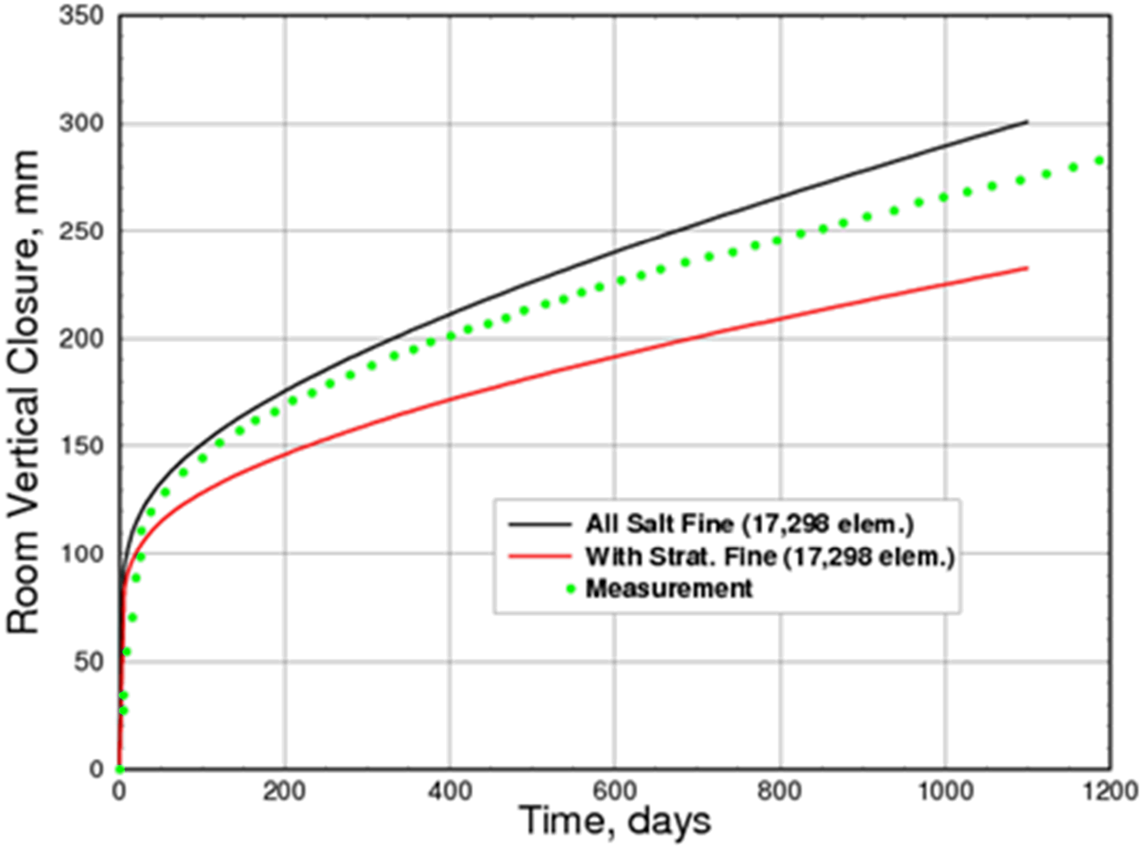

Figure 5. Room D Vertical Closure Results with “Refined” Mesh Compared to Measurements

Given that a significant difference in computed results with an ~8X refinement was seen, we needed to establish, if indeed, the calculational vertical closure results had converged with mesh refinement. To this end, we took the full-stratigraphy case this current FY and performed a limited study of the continued refinement of the mesh. Only a limited study was performed due to time/budget limitations and computational difficulties as the mesh size grew large.

The mesh was refined to two finer levels – first to 29,748 elements (~14X the coarse mesh) and then to an even finer 81,042 elements (~37X the coarse mesh). Figure 6 shows the results of this limited study. The computed vertical closure continues to change as the computational mesh is refined, with the differences in computed vertical closure diminishing with greater refinement, as seen in the figure. However, even at the last two refinement levels, we still see a difference of about 2.5% in the computed vertical closure at the end of the 1100 day simulations between these two levels (0.239 m with the 29,748 element mesh vs. 0.245 m with the 81,042 element mesh). This implies that a final converged mesh may not yet have been reached, because in theory, once a final converged refinement level is reached, the computed vertical closure should not change with further refinement. It appears that at the end of the 1100 day simulation, the solution may converge to a value of ~0.25 m, but it is not there yet. Furthermore, even the finest mesh still produces computed results that appreciably under-predict the measured values. The reasons for this remaining difference need to be investigated to determine their origin, but could be due in part to the parameter uncertainties (e.g., coefficient of friction used in the sliding interfaces & the creep parameters used for salt) and the changes made to the stratigraphy by Munson et al. (1989), from the reference stratigraphy proposed earlier by Krieg (1984).

It should be noted that the sharp corners of the Room D model may be contributing to the mesh convergence difficulties seen here and a modification of the computational model to incorporate rounded corners may be needed. The rounded corners would help eliminate the very high gradients seen in the sharp 90° corners of the room. To this end, it is recommended that a formal mesh refinement study of the Room D simulations be completed with whatever computational model is finally used for Joint Project III.

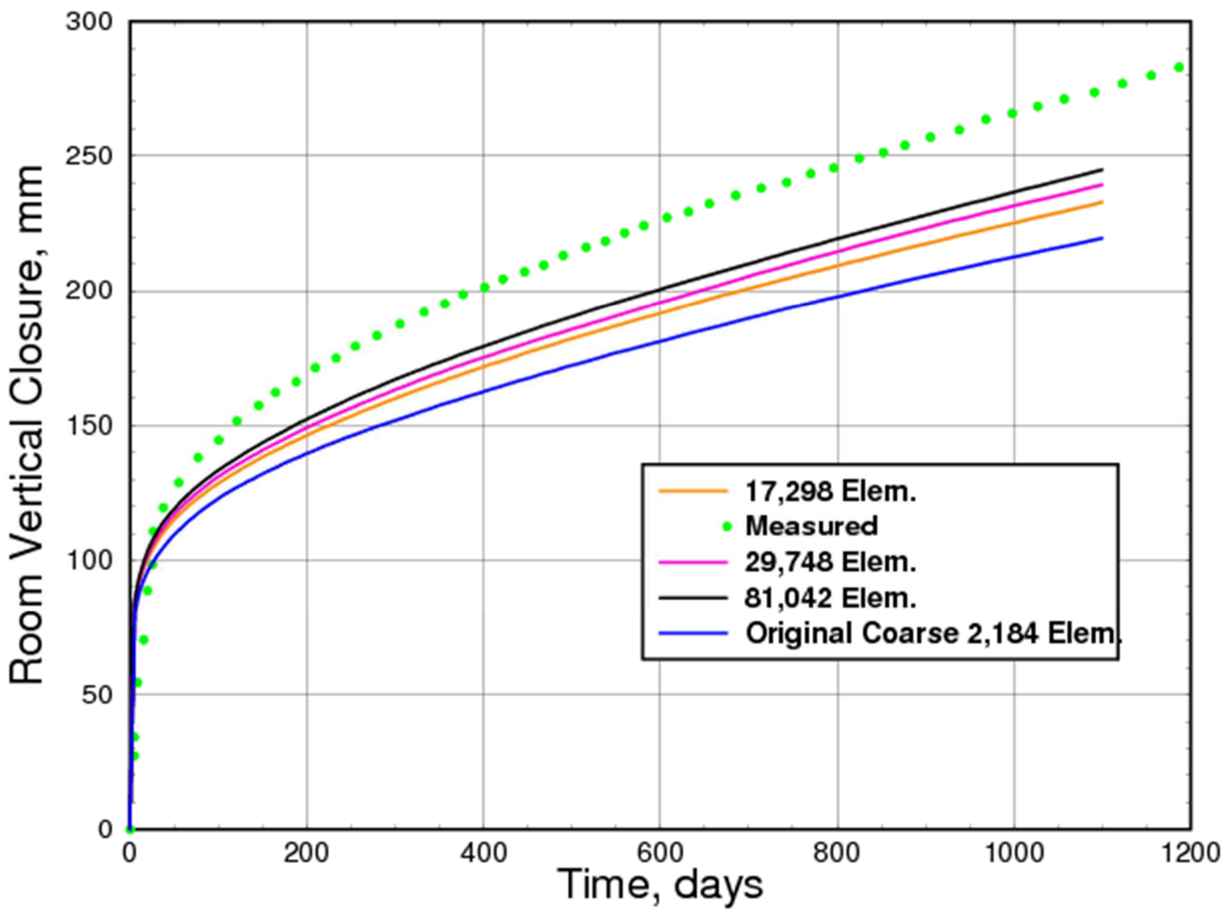

Figure 6. Full Stratigraphy Case of Room D Vertical Closure Results with Continued Refinement of the Mesh

All-Clean-Salt Calculation & Effect of Not Including Sliding at the Clay Seams – Two additional calculations that were performed this current FY were one in which the configuration was treated as being comprised of all-clean-salt (as opposed to one containing both clean salt and argillaceous salt), with the nine clay seams nearest the room included in the model as being active sliding surfaces and another with all-clean-salt, but with the clay seams of Room D not included as sliding interfaces. As mentioned previously, the legacy model includes either all-salt (both clean and argillaceous salt) or the full stratigraphy, with the effects of potential sliding at the nine clay seams nearest the room using sliding interfaces to represent them.

However, the German partners, under the Joint Project III benchmarking effort have chosen to do an all-clean-salt calculation and to not include the clay seam sliding in their preliminary model of WIPP Room D. This is being done by the German partners because they found from their laboratory testing of WIPP salt that the differences between the mechanical behaviors (creep rates) of the WIPP clean salt samples and the WIPP argillaceous salt samples that they tested did not differ significantly from one another. Furthermore, the testing of actual clay seams to determine an appropriate value of friction coefficient has never been undertaken. The friction coefficient value used in the legacy calculations of Munson (1997) was arbitrarily taken as 0.2 because it was considered a “free” parameter (Munson et. al 1989).

Consequently, this pair of calculations was undertaken to quantify how the magnitude of vertical closure would change in an all-clean-salt configuration with and without sliding at the clay seams. So one of these calculations used the same assumptions used by the German partners. In addition, the other calculation, with the presence of the sliding at the clay seams, was performed to quantify how much additional vertical closure would result due to the sliding at the clay seams. It should be noted that this is the first time, to the author’s knowledge, that we have modeled WIPP Room D assuming an all-clean-salt configuration using the clean salt parameters shown in Table 1. Figure 7 shows, the results of the new calculations with an all-clean-salt configuration. The first one without the clay seams actively sliding is designated as “Slidelines Fixed.” The results of this one can then be compared to the second case with the slidelines included and designated as “Slidelines Active.” Both of these calculations used the model with the 17,298 element mesh.

Figure 7 shows that for the “equivalent” German partner case (“Slidelines Fixed”), the vertical closure of the room at the end of the 1100 day simulation is ~0.140 m, which is significantly less than the ~0.300 m computed with the all-salt (both clean and argillaceous) calculation, shown in Figure 5. Furthermore, allowing the slidelines to move (“Slidelines Active”) results in only about 0.04 m of additional vertical closure (~0.180 m at 1100 days). This latter calculation is the one most directly comparable to that shown in Figure 5 for the all-salt calculation, with the only difference being the use of all-clean-salt in the configuration (Figure 7) as opposed to the use of both clean and argillaceous salt (Figure 5). Note that both of the calculations shown in Figure 7 would result in the significant under-prediction of the measured room vertical closure. Consequently, it appears that the higher creep rates (“structure factors” in Table 1) recommended by Munson (1997) for the argillaceous salt are values that have been adjusted in the computational model, along with the coefficient of friction in the slidelines, to match the measured vertical closure. However, the legacy calculations also appear to have used a relatively coarse mesh in the computational model – one that is way too coarse by today’s standards and one that with further refinement will lead to differing results as it is refined. This should provide further impetus for completing a formal “mesh-refinement” study that will lead to a viable computational model that is sufficiently refined for convergence and use in the benchmarking calculations of Joint Project III.

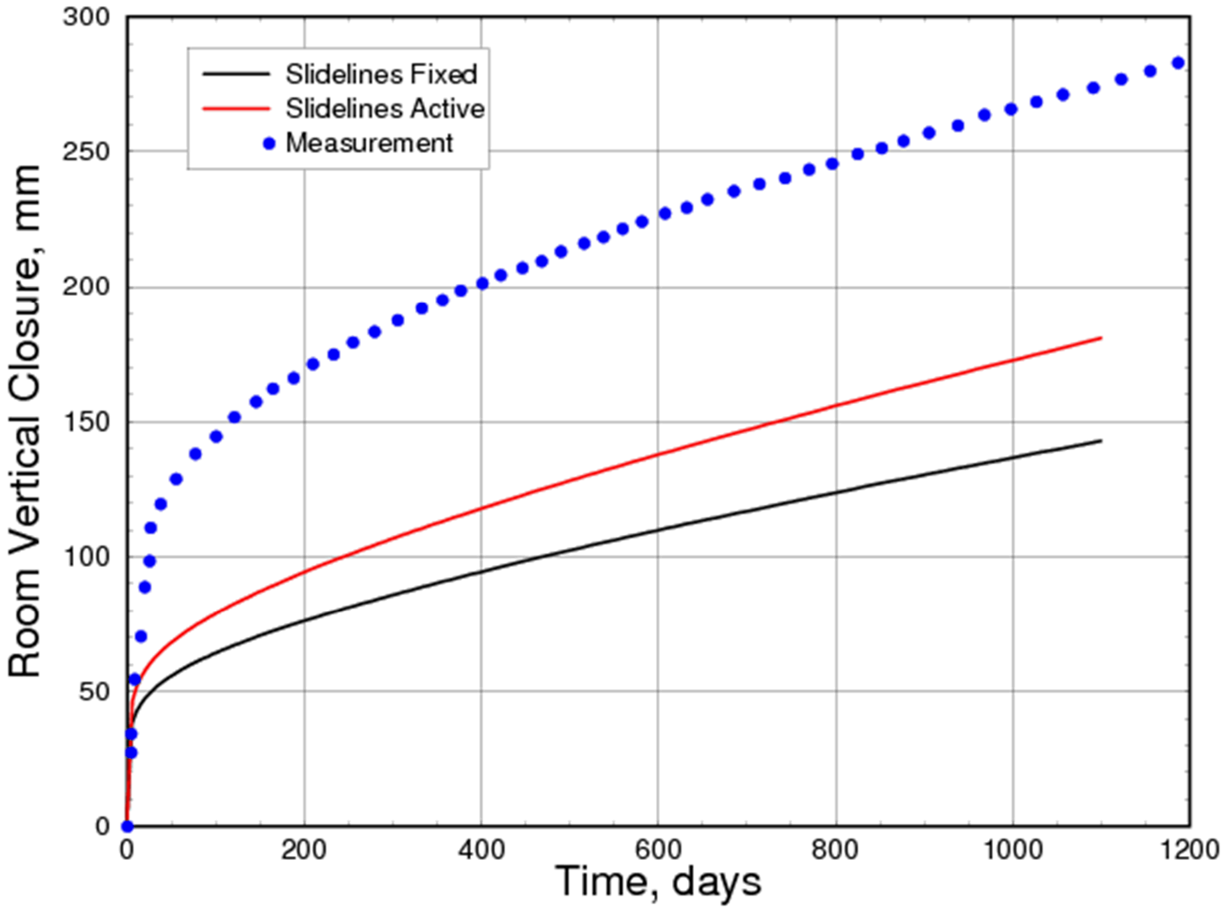

Figure 7. All-Salt Case of Room D Vertical Closure Results With and Without Slidelines Active in the Calculation – Compared to the Closure Measurements

5. PARTICIPATION AND PRESENTATION AT SALTMECH VIII

The author participated with an article (Argüello & Holland 2015) and presented on "Two Problems for Benchmarking Numerical Codes for use in Potential HLW Salt Repositories" (SAND2015-4053C) at the Eighth International Conference on the Mechanical Behavior of Salt (SaltMech VIII), at the end of May in Rapid City, SD. In introducing the problems the author first talked about how 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. He further discussed that 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. The author also noted that significant advances have been made in both the hardware and the computational software available to model potential HLW repositories in salt. He noted that 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. The detailed definitions of two benchmark problems were then presented that are consistent with idealizations of two WIPP in-situ full-scale underground experiments – WIPP Rooms B & D. The author noted that it is hoped that the benchmark problems defined in the article will be useful to the salt community at large and allow others to benefit from their availability. He also noted that these problems, or ones similar to these, can be used to assess the current generation of computational software available for modeling potential HLW repositories in rock salt, for example in the U.S.-German Joint Project III. The author then presented select results from several preliminary calculations carried out for the isothermal WIPP Room D. These included results for the problem, as defined, as well as possible variants to the defined problem.

The conference itself overall included several topics of interest to the salt community at large: Laboratory Testing; Field Applications; Barriers; Solution Caverns; Constitutive Modeling; and Modeling & Simulation. Of special note was the high visibility of the U.S.-German Joint Project III, with a total of six contributed papers at the conference that were related to the Joint Project efforts. This was six out of forty-four total papers that were contributed to the conference and included: Salzer et al. (2015), Düsterloh et al. (2015), Hampel (2015), Argüello & Holland (2015), Gährken et al. (2015), and Hampel et al. (2015).

6. EIGHTEENTH JOINT PROJECT III MEETING

The author participated the 18th quarterly project meeting of the U.S.-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 South Dakota School of Mines and Technology in Rapid City, SD. Lance Roberts, Frank Hansen, and the author served as co-hosts of the meeting. Because this meeting was in Rapid City this time (typically held in Germany) and was held immediately after SaltMech VIII, it facilitated having additional attendees from the U.S. at this meeting from both Sandia and RESPEC.

The meeting started off with an introduction of the various participants, given that there were additional people from the U.S. In particular, Ben Reedlunn was introduced to the group - he will continue to lead the Joint Project III work on the U.S. side upon the author's upcoming retirement. Because of the additional U.S. participants, a review of the previous work carried out under Joint Project III was presented by Andreas Hampel to bring everyone up-to-date and set the stage for the present discussions. This included a discussion of the benchmarking efforts on two borehole tests that were performed at the Asse in Germany, the so-called Isothermal Free Convergence (IFC) test and the Heated Free Convergence Probe (HFCP) test. Both tests were conducted in the same nominal 31.5 mm diameter borehole that was drilled from a working chamber approximately 750 m below the surface within the salt dome. The two tests were at different depths from the floor of the working chamber. The IFC was at a depth of 292 m below the chamber floor, and the HFCP was at a depth of 231 m below the chamber floor. The results from the benchmarking efforts on these two tests are reported in Hampel et al. (2013).

The work done under Joint Project III on the Dammjoch "test" was discussed next. The Dammjoch is another instance of a structure in the Asse. A drift was mined at a depth of approximately 700 m, in the 1910's – later a portion of the drift was lined with a cast iron liner and the space between the liner and the salt in the drift wall was filled-in with concrete. After approximately 85 years of the liner being in-place (in 2001), the permeability was measured in the salt adjacent to the drift in both the lined and unlined sections. The permeability in the lined section was found to be orders of magnitude smaller than in the unlined section, providing evidence that salt "heals" in the excavation damage zone (EDZ) when there is resistance to the convergence of the drift, such as that provided by the liner. The EDZ adjacent to the opening was originally created when the drift was mined. The results of Joint Project III benchmarking efforts on the Dammjoch were reported in Hampel et al. (2015).

The current efforts under Joint Project III were the next topic discussed, namely an overview of the work currently being performed to model the full-scale in-situ WIPP Rooms D and B tests. These tests were both carried out in the early-to-mid 1980's at the WIPP near Carlsbad, NM, U.S. As opposed to the previous tests, which were in domal salt, Rooms D and B were in bedded salt. A series of laboratory tests have been performed by the German partners under Joint Project III on WIPP salt from salt core provided by the U.S. Results from this testing program have been reported by Salzer et al. (2015) and Düsterloh et al. (2015). The laboratory testing program conducted by the Germans on WIPP salt indicated that there were only minor differences in the mechanical behavior (creep response) of clean vs. argillaceous WIPP salt. In fact, in Hampel's CDM model, the parameters used for both the clean and argillaceous WIPP salt are the same.

Andreas Gährken gave an overview of the results of the partner's WIPP Room D calculations to date. The first case considered is a configuration for WIPP Room D that is an all-clean-salt configuration with all of the sliding surfaces fixed against movement (essentially neglecting sliding at any of the clay seams). The results from these simulations showed a general agreement among the results of the various German partners with one another (although there was some scatter) in terms of vertical closure results, and these significantly under-estimate the measured vertical closure of the room. The only exception to this trend was the results from KIT, but they did not follow the specifications of how the problem should be run, so this was not unexpected.

The author shared the results of his all-clean-salt calculation (comparable to the one run by the German partners and described in the previous section) that also showed a significantly smaller vertical room closure compared to the measurements. So it appears that the argillaceous WIPP salt parameters used by Munson (1997), which are significantly different from the clean WIPP salt parameters along with the effects of sliding at the clay seams, play an important role in the agreement that he reported with the measurements.

A second case that the German partners are also planning to run is a configuration that includes the various layers of the stratigraphy. This will include a Mohr-Coulomb material model used for the anhydrite and a power-law plasticity model used for the polyhalite, but still with all sliding surfaces fixed.

The next order of business was a discussion of a follow-up to Joint Project III. Joint Project III is to finish by early 2016, and there is a need and desire from both sides to continue collaborative work in the wake of the progress that has been made in the joint project. Several topics have been under discussion by the various participants in Joint Project III since before the 5th U.S.-German Workshop in Santa Fe. However, after much discussion amongst the partners, the list of potential follow-on topics is:

- Continued assessment and investigation into deformation behavior at small deviatoric stresses such as might be typical in repository setting;

- Deformation behavior resulting from tensile stresses;
- Influence of inhomogeneities such as might be found in bedded salt (layer boundaries, interfaces) on the deformation; and
- Influence of temperature and stress state on the damage reduction.

Among the discussion related to these topics, Savas Yildirim raised questions on the issues relative to the behavior at lower deviatoric stresses, noting the work of Pierre Bérest at creep rates 0.5-0.2 per day. How does this relate to the long-term safety of the repository and the construction of closures or seals. Klaus Salzer briefly talked about testing of salt at 0.002 /day rate noting that dislocation density is about the only thing that one can measure – he also talked about deformation behavior resulting from tensile stresses and how to quantify that. Christian Missal briefly talked about influence of boundary planes on the deformation of rock salt. Kai Herchen briefly talked about the importance of damage reduction for repositories in rock salt and also about knowledge deficits and planned work on damage reduction in rock salt.

The next (19^{th}) meeting for the Joint Project III participants was set for July (Thursday & Friday) 23-24 in Braunschweig. Because of the relatively brief period before this next meeting, only the German partners will participate. Participation by the U.S. in the next Joint Project III meeting will be before or after the 6^{th} U.S.-Germany Workshop in Dresden (Sept 7-11, 2015), with tentative dates of the 5th and 6th of September for the 20^{th} Joint Project III meeting.

7. SUMMARY

Various activities continued in the area of international benchmark calculations of field experiments during FY15. The work is being carried out under the auspices of a U.S.-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 <u>domal</u> salt, Joint Project III was extended (with funding from the BMWi on the German side) to include two additional problems in <u>bedded</u> salt: WIPP full-scale in-situ test 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. They have completed their laboratory testing of both the clean and argillaceous WIPP salt and found relatively small differences between the two.

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 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. Furthermore, this FY's efforts show that with two additional refinement levels, the computed results are still changing and that it is likely that a converged mesh for the problem has not yet been reached. This finding points to the need for a formal mesh-refinement study to arrive at such a converged computational model. Furthermore, this implies that in the legacy model of the rooms and calculations, the MD parameters (and other features of the model, such as the friction coefficient used in the sliding of the clay seams) were calibrated to match the tests using a relatively coarse mesh that was acceptable at the time, but that now appears much too coarse. This is an issue that we hope to address under Joint Project III. An appropriate refinement level for the mesh used in the calculations needs to be determined from a formal mesh-refinement study. Once this is done a common refinement of the room among the partners will likely be needed to make appropriate comparisons between the results of the various partners participating in the benchmark exercise.

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