

Exceptional service in the national interest



Modeling WIPP Rooms D and B



J. Guadalupe Argüello

5th International US-German Workshop on
Salt Repository Research, Design and
Operation

Santa Fe, NM September 2014



Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2014-XXXXP

Benchmarking WIPP Rooms for JP III

- “Joint Project III” was extended to include two additional benchmarking problems based on in-situ full-scale tests conducted in the early 1980’s at the Waste Isolation Pilot Plant (WIPP), located in Southeastern New Mexico, USA
 - The isothermal Mining Development Test – WIPP Room D
 - The heated Overtest for Simulated Defense High-Level Waste – WIPP Room B
- Work on WIPP salt (lab tests and Rooms D & B) is again related to temperature dependence and is thus an extension of the first benchmarking problem
 - Larger rooms
 - Quadrilateral cross-section
 - More importance of damage (at least at corners and possibly roof)
 - At different temperatures than in IFC & HFCP tests

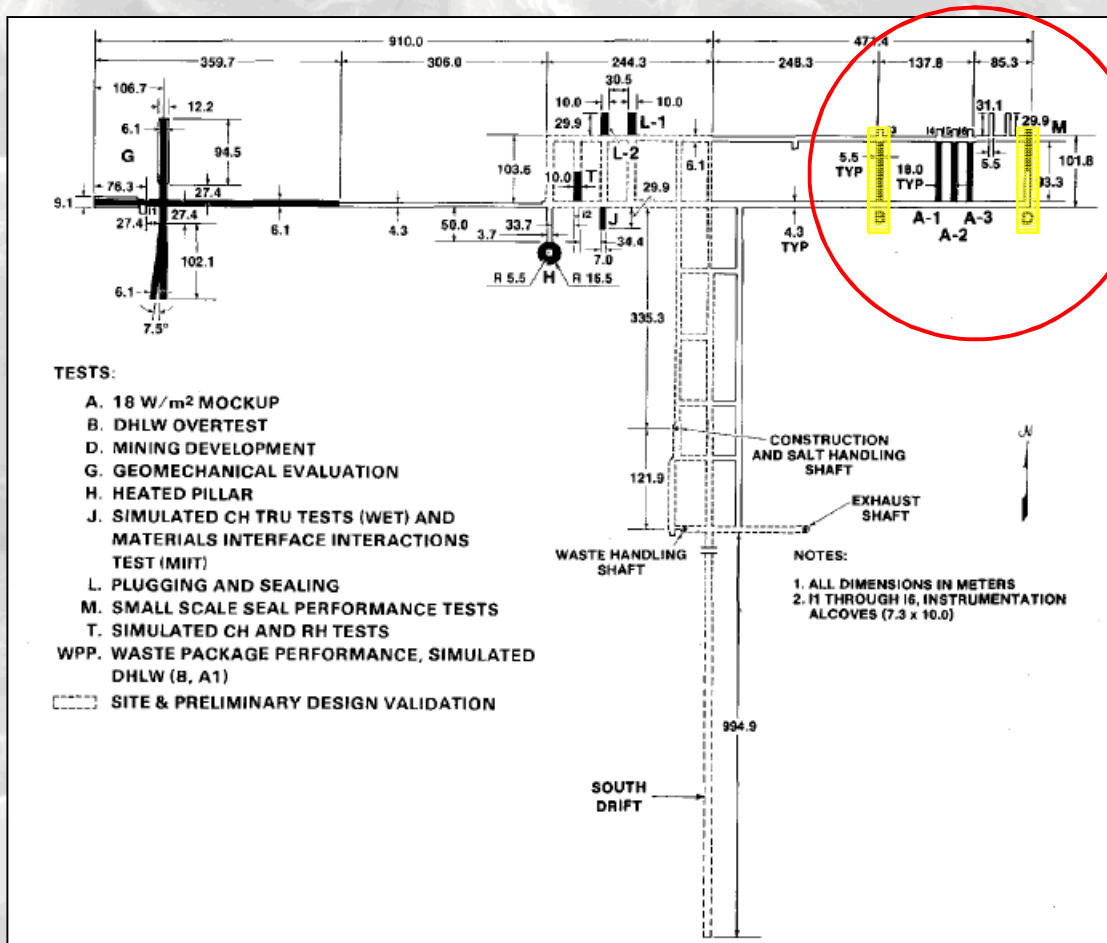


Room D



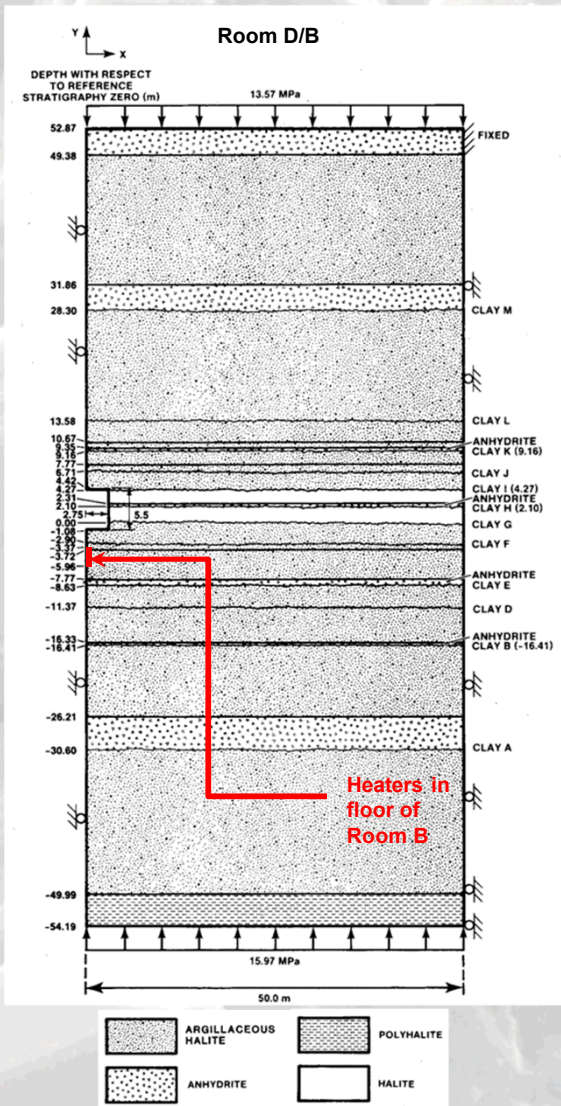
WIPP Experiments of Early 80's

Several Thermal-Structural Interactions (TSI) Experimental Rooms Fielded at the Waste Isolation Pilot Plant (WIPP) in the early 80's



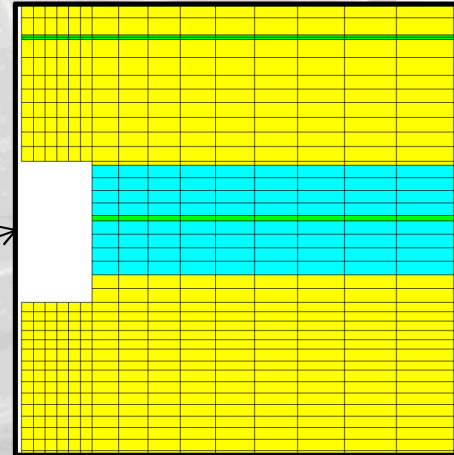
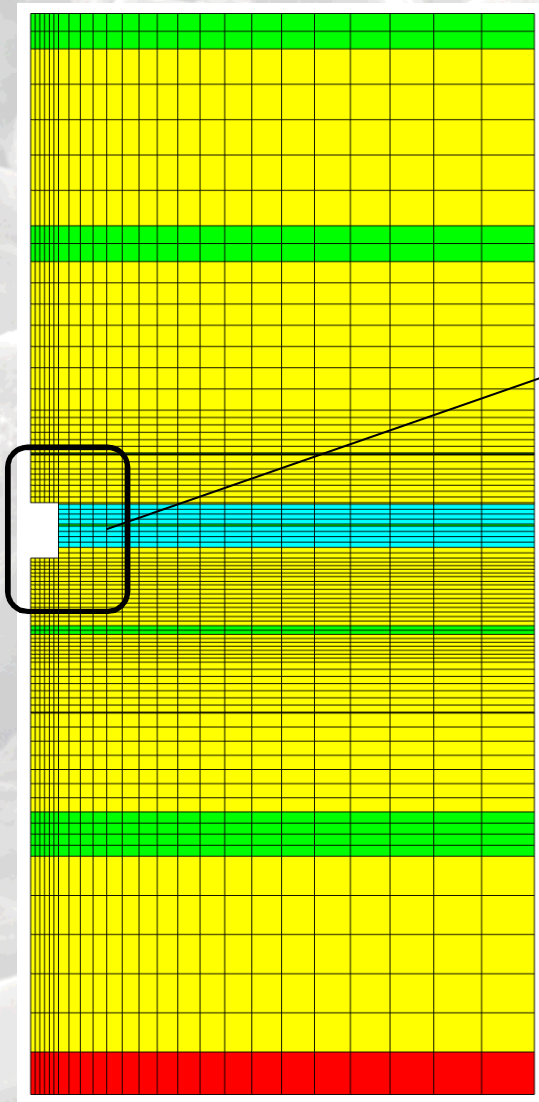
Experimental WIPP Rooms D & B are of special interest & well-suited for benchmarking

Why are WIPP Rooms D & B Well-Suited for Benchmarking?



- **Except for the heat load in Room B, both rooms are essentially identical**
 - Located in the same general area of WIPP
 - Relatively “isolated” from other workings
 - 5.5 X 5.5 m in cross-section (~100 m long)
 - At the same horizon and thus in the same vertical stratigraphic location
 - Tests conducted under rigorous Quality Assurance
 - Gages calibrated to NIST standards
 - Were extensively instrumented and data were taken for approximately 3.5 years (1300-1400 days) after excavation
 - Comprehensive datasets archived and available for benchmarking efforts

WIPP Room D Coarse Mesh



Coarse FEM mesh used originally with Sierra Mechanics transmitted to German partners:

- 5032 nodes & 2184 hexahedral elements
- 4 element blocks – halite, argillaceous halite, anhydrite, & polyhalite
- 9 clay seams nearest room included as sliding surfaces
- Traction of 13.57 MPa at top & 15.97 MPa at bottom of model
- Roller B.C.s on both sides and Fixed B.C. near top right

Mechanical Modeling Parameters for Use in WIPP Room D/B Calculations

Note: Models based on details provided in Munson, 1997, *Int. J. Rock Mech. Min. Sci.* 34:2 233-247 (& supplemental information not provided there)



- Clean salt and **Argillaceous** Salt modeled with MD creep model with parameters shown here

	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	

Mechanical Modeling Parameters

(Cont'd)

- Anhydrite and Polyhalite modeled with an elastic/perfectly-plastic Drucker-Prager criterion: $F = \sqrt{J_2} + aI_1 - C$

where

$$I_1 = \sigma_{kk}$$

$$J_2 = \frac{1}{2}S_{ij}S_{ji}$$

a, C = material constants



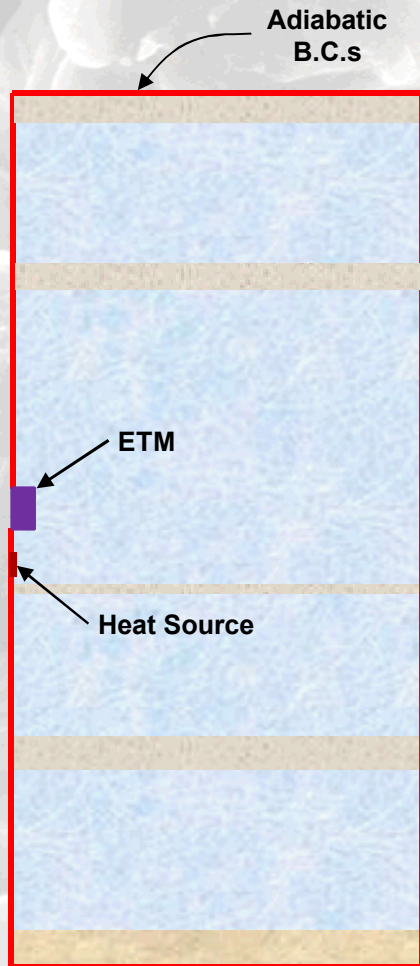
with parameters as shown in table below.

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



- Clay seams modeled as sliding surfaces with M-C behavior: $\tau = \mu\sigma_n$ with $\mu=0.2$
- Initial stress set to lithostatic stress varying linearly with depth

Thermal Modeling Parameters for Use in WIPP Room B Calculations



- All boundaries in “red” assumed to be adiabatic
- Boundaries sufficiently remote to preclude affecting room response for duration of simulation
- Entire formation prescribed to have an initial temperature of 300 K
- The drift area (in “purple”) assumed to consist of an “equivalent thermal material” (ETM)
- ETM has a constant high conductivity of 50 W/(m-K) & a high thermal diffusivity [C_p of 1,000 J/(kg-K) and a density of 1 kg/m³]
- This presumably simulates radiative heat transfer in the room by an equivalent conduction
- Clay seams to be neglected in thermal analyses

Thermal Modeling Parameters (Cont'd.)

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

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

where λ is the thermal conductivity, T is the absolute temperature in Kelvin, and λ_{300} & γ are material constants.

The various parameters are given in table below and include:

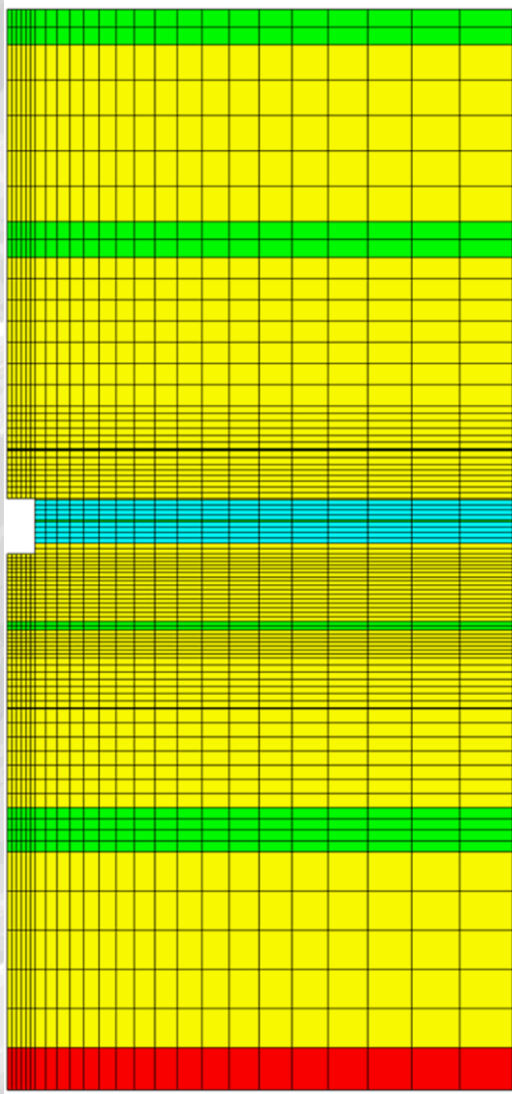
C_p – the specific heat;

α – the coefficient of linear thermal expansion; and

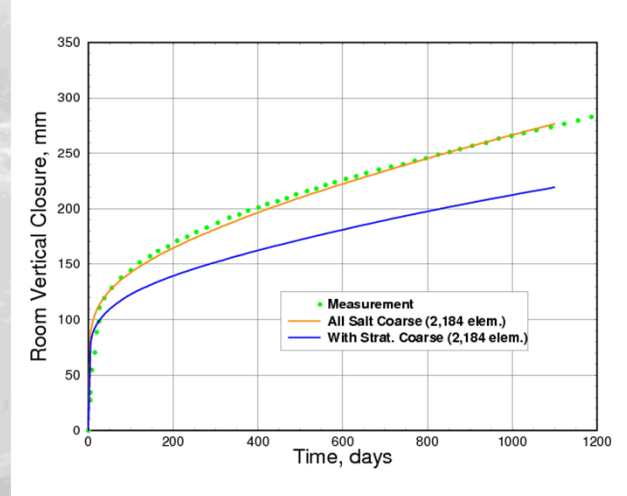
ρ – the material density.

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

Room D Model Matching Capability Available in Mid-80s to early 90s

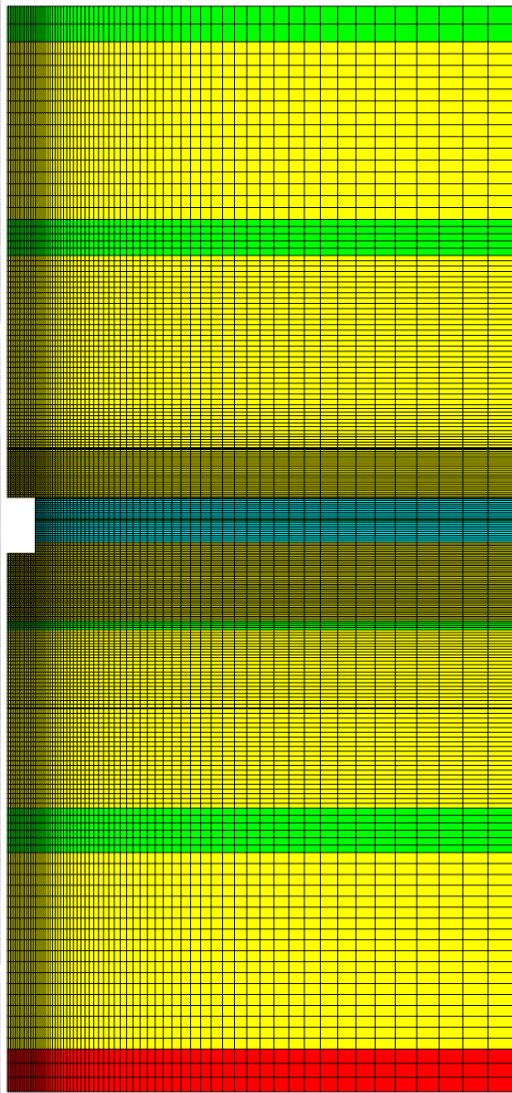


Original Mesh

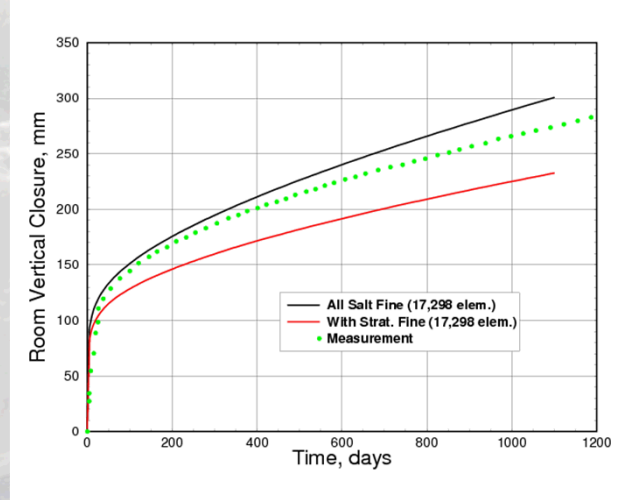


- Original mesh coarse by today's standards, but similar to what was possible in the mid-1980s to early 1990s, in terms of computational capability
- With this mesh, computed vertical closure comparable to measured values (using all-salt stratigraphy, as apparently done in past)
- With this mesh and the complete stratigraphy, computed vertical closure is less than the measured closure

Refining the Room D Model in Line with Current Generation Capability



Refined Mesh



- New generation of computational tools allows more refined mesh, in line with current practice/ standards, to better-capture stress gradients
- Mesh shown here includes ~8X the number of elements as the coarse mesh (not possible with machines of mid-80s to early 90s)
- With refined mesh, computed vertical closure is greater than that computed with coarse mesh, for either the all-salt or with complete stratigraphy cases
- Computed results bracket the measurements

Summary & Conclusions

- Initial efforts on WIPP Room D underway
- Original coarse mesh with various details transmitted to German partners
- Additional information needed for the benchmarking effort has been identified and will be transmitted
- Using original mesh with all-salt idealization, the computed Room D vertical closure with SIERRA Mechanics agrees reasonably well with the measurements
- Refinement of Room D model to conform with modern standards/practice leads to greater vertical closure than measurements for the all-salt idealization but less than measurements for the full stratigraphy
- Appears that in legacy model, MD parameters (& other features, e.g., μ for clay seams) were calibrated to match the tests using a relatively coarse mesh acceptable at the time
- This remains an open question that we hope to answer under JPIII
- Implies that a common refinement of the room model among the partners may be needed to make appropriate comparisons among the results of the various partners participating in the benchmark