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PROGRESS IN VALIDATION OF STRUCTURAL CODES FOR RADIOACTIVE WASTE REPOSITORY APPLICATIONS IN BEDDED SALT*

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PROGRESS IN VALIDATION OF STRUCTURAL CODES FOR RADIOACTIVE WASTE REPOSITORY APPLICATIONS IN BEDDED SALT (1)

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ABSTRACT

Over the last nine years, coordinated activities in laboratory database generation, constitutive model formulation, and numerical code capability development have led to an improved ability of thermal/structural codes to predict the creep deformation of underground rooms in bedded salt deposits. In the last year, these codes have been undergoing preliminary validation against an extensive database collected from the large scale underground structural in situ tests at the Waste Isolation Pilot Plant (WIPP) in Southeastern New Mexico. This validation exercise has allowed the prediction capabilities to be evaluated for accuracy. We present here a summary of the predictive capability and the nature of the in situ database involved in the validation exercise. The WIPP validation exercise has proven to be especially productive.

RÉSUMÉ

Ces neuf dernières années, des activités coordonnées de production de base de données de laboratoire, de formulation de modèle constitutif et de développement des possibilités des codes numériques ont abouti au perfectionnement des capacités des codes thermiques/structurels visant à prédire le fluage des chambres souterraines dans les couches de sel de noyage. Au cours de l'année passée, ces codes ont subi une validation préliminaire par rapport à une base exhaustive de données rassemblées à partir d'essais souterrains à grande échelle, in situ, réalisés à l'usine pilote d'isolation des déchets (Waste Isolation Pilot Plant - WIPP), au sud-est du Nouveau Mexique. Cet exercice de validation a permis d'évaluer le degré de précision des capacités de prédiction. Nous présentons ci-après un résumé des capacités de prédiction et la nature de la base de données in situ sur lesquelles l'exercice de validation s'est fondé. Cet exercice de validation à la WIPP s'est avéré être tout particulièrement fructueux.

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INTRODUCTION

The purpose of the Waste Isolation Pilot Plant (WIPP) Project is to develop a technology base for underground disposal of radioactive Transuranic (TRU) waste from the U.S. defense projects in a bedded salt deposit. One requirement is to assure that the repository will isolate the waste from the biosphere until it is no longer a threat to man. In salt, isolation depends in part upon the creep of the salt to aid in sealing the repository and encapsulating the waste. As a result, a predictive technology for the structural behavior of salt must be developed to determine response of repository seals and closure time of the rooms. The extremely large forward extrapolation in time of the prediction places demands on the technology that greatly exceed previous engineering practice. In general, overall technology development is the responsibility of Sandia National Laboratories, with the Thermal/Structural Interactions (TSI) program specifically organized to address the structural aspects.

As originally defined, the TSI program approach to a predictive capability was based on a mathematical model of constitutive behavior and laboratory determination of relevant material parameters. The model was to be based on first principles, where possible, or laboratory empirical inputs, as necessary. Results from in situ testing at the WIPP facility would be used as final validation of the predictive technology, not as a database for obtaining backfitted solutions [1]. Separation between the independently developed predictive capability and the means of validation is considered essential to the requirements of a radioactive waste disposal technology.

Technology demonstration implies compliance with the Environmental Protection Agency (EPA) regulations. To demonstrate the repository technology in anticipation of establishing a repository, a pilot plant facility has been constructed in salt, 659 m underground, in southeastern New Mexico. This facility also provides a setting for the large-scale, in situ tests which are supplying part of the databases for technology development and validation.

It is the intent of this paper to show our progress in the development of the structural predictive capability and the results of initial validation comparisons between calculations and in situ test data.

STRUCTURAL RESPONSE PREDICTIVE TECHNOLOGY

To permit orderly calculations for project needs, an initial reference creep law, together with reference material properties and stratigraphy, was established by 1984 [2]. These reference conditions did not preclude further development of more sophisticated creep models or updates in material creep properties and stratigraphic representations. The 1984 reference was based on a thermally activated, steady-state function (with a seldom-used, first-order kinetics, transient representation) compatible with integration schemes of existing numerical codes at that time. Material properties were determined from laboratory creep tests of core specimens obtained from deep boreholes at the proposed WIPP site, and the stratigraphy was constructed from core descriptions from the same deep boreholes at the site. While existing code capabilities were being used for repository and in situ test parametric studies, these codes were also undergoing benchmark exercises against boundary value problems intended to verify their numerical adequacy [3]. However, benchmark verification exercises are insufficient to guarantee code accuracy for the highly nonlinear constitutive models believed representative of the behavior of salt; thus, confidence in prediction technology depends in part upon validation against the extensive in situ database now becoming available.

In the first comparison of calculations using the 1984 reference conditions and actual in situ closure data from the South Drift, Morgan et al. [4] found that the calculations underpredicted the closure and closure rates by a factor of three. Further examination revealed that the known uncertainty in material properties did not permit enough variation to explain the results [5]. A fundamental resolution of this discrepancy was essential to the development of an acceptable predictive capability. The resolution effort has resulted in an extensive reevaluation of the entire predictive technology.

REEVALUATION STUDIES

In a preliminary effort to determine the relative influence of the various aspects of the predictive technology, Munson and Fossum [6] used a multimechanism, steady-state creep model with a workhardening/recovery transient response, and two different flow potentials. These results suggested the importance of the stress generalization (flow potential), the need for a precise description of the transient creep, and the significance of omissions of important strains from the creep generated databases.

Flow potential: The flow potential is the significant factor in extending laboratory creep data obtained in uniaxial stress tests to any generalized, three-dimensional calculation. Various representations of the flow potential, even though they degenerate to the same value in uniaxial stress, can vary greatly for other stress states. This difference in flow potential is exaggerated in calculations of creep closure because the creep rate is a very strong function of the stress. Investigation of the flow potential for salt creep was undertaken using laboratory tests of thin-walled cylindrical specimens. As a result of these tests, it appears that a maximum shear stress or Tresca criterion better describes the flow surface [1], in contrast to the assumption of a von Mises criterion used previously [2].

Constitutive model: Initially, a common assumption was that for long-term creep closure of the rooms, only steady-state creep behavior needed to be considered. However, this was questioned on the basis that strain, not time, governs achievement of steady state. As the stress field around the rooms expands with time (for the WIPP configuration), large volumes of previously unstressed salt progressively come under stress. As a result, there are always large volumes of previously unstrained salt undergoing the pronounced transient strains exhibited by salt. These transient strains in the new material encompassed by the expanding stress field contribute significantly to the integrated room closure displacements, even though the stresses producing the strains may be small. Thus, inclusion of the proper description of the small strains of transient creep into the constitutive model is essential.

The constitutive model currently used by the Project is based on the deformation-mechanism map specific to the expected WIPP conditions. As most recently modified [1], this constitutive model (modified M-D model) consists of multimechanism, steady-state creep with a workhardening/recovery transient creep response, treats recovery (stress unloading), and includes a quadratic approximation to the small strain portion of the transient response. The model includes three distinct mechanisms: (1) a dislocation climb mechanism at high temperatures, (2) an undefined (but empirically well specified) mechanism at low stresses and temperatures, and (3) a dislocation slip mechanism at high stresses, all acting in parallel. The modified M-D constitutive model is used in all of the preliminary validation calculations presented here.

In addition to the salt layers, bedded natural evaporite deposits also contain substantial layers of anhydrite. As initially defined by Krieg [2], the time-independent deformation of the anhydrite is described through a Drucker-Prager yield function. This description has been retained for the preliminary validation calculations.

The shear response of clay seams commonly found in bedded evaporite deposits is accommodated through incorporation of slip lines in the numerical codes. Shear along the slip lines is governed by Coulomb friction [2].

Material parameters: The emphasis on small strain response resulted in reevaluation of the methods for determining material parameters. The reevaluation centered on including previously ignored "lost" strains into the parameter determination. In the past, parameters were typically determined from laboratory creep tests, where time and strain are rezeroed when the loading to the stated stress level is complete. Consequently, creep databases exclude the significant, although small, loading strain associated with creep testing. In addition, creep specimens are obtained from either deep boreholes or from around underground excavations into the "virgin" salt beds. Under these conditions, specimens can accumulate excavation strains prior to testing which are not recaptured by the laboratory testing. In order for the material parameters to correctly reflect the excavation of the WIPP facility from virgin salt beds, these loading and excavation strains must be included in the database from which the parameters are determined [1,6].

Based on the reevaluation, two major bedded salt layer types are evident, clean salt and argillaceous salt, for which new material parameters are determined. For the anhydrite layers, the Drucker-Prager constants are determined from laboratory quasi-static compression tests. The coefficient of friction of clay seams cannot be determined in the laboratory and reasonable values must be assumed. This process leads to the reevaluated parameter set used in the calculations, as given elsewhere [1]. At this time, only the coefficient of friction parameter of the required parameters cannot be defined through laboratory tests, and remains a free parameter.

Stratigraphy: Although too complex to describe here, the reevaluation of the stratigraphy based on underground observations indicates significantly more beds consist of argillaceous salt than the 1984 reference stratigraphy [2] indicated. The current stratigraphy [1] reflects this difference.

IN SITU TESTS

A number of test rooms and room complexes have been excavated in the underground facility, as shown in Figure 1. Available structural validation tests are summarized in Table 1. The structural response of these tests is being measured to create the in situ test database required for the validation exercise. The intent is to measure the salt displacements around the test rooms in exceptional detail from the first moment of excavation. However, measurements in some of the early excavations were outside the research effort and did not meet this intent. In these cases, it is necessary to reconstruct the early, lost displacements. The test rooms or room complexes represent a number of different geometries, including a circular cross section room, with individual rooms situated in three somewhat different stratigraphic settings. Also, two of the four shafts have been well instrumented at as many as five discrete horizons in the salt.

Although data continue to be gathered from these tests, the database is already very extensive, with sufficient data to permit meaningful comparison to preliminary validation calculations. At this time, we have completed calculations of the isolated, single test rooms or drifts, which we report here. The complex multiple room configurations which represent somewhat more difficult calculations are now under study, so these calculations will be forthcoming.

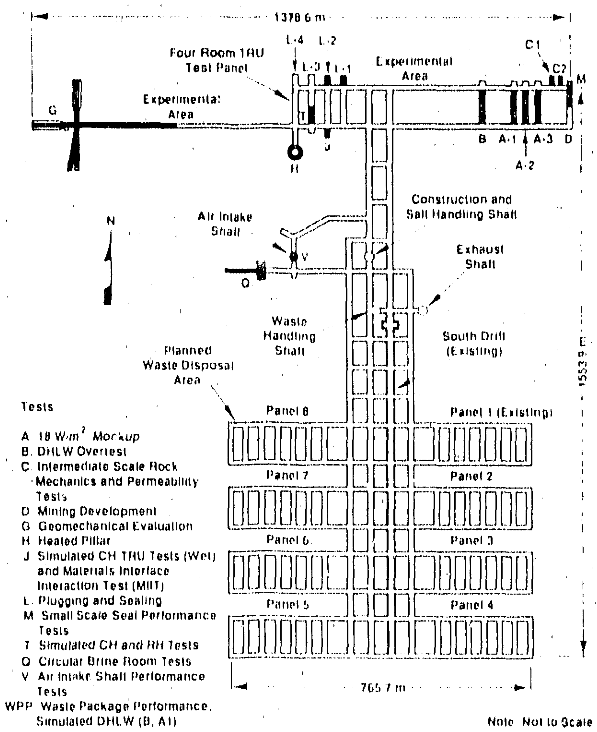

Figure 1 Plan View of the WIPP Underground Facility

PRELIMINARY VALIDATION CALCULATIONS

Although the South Drift represents the first underground excavation to be compared to calculation with the previously noted three-fold prediction discrepancy [4], it was not the first of the current preliminary validation calculations using the M-D model and reevaluated parameter set. Preliminary validation efforts initially focused on Room D, where closure measurements were taken at gage stations within an hour of excavation of the virgin salt. The attention to obtaining very early displacements for the in situ validation database is the equivalent of incorporating all specimen strains in the database for parameter determination, which assures both databases correspond to "virgin" conditions. The Room D calculation as reported by Munson et al. [1] used the reevaluated parameter set and stratigraphy (Set A), except for a few minor differences. This calculation used a 40% larger value of transient strain limit for argillaceous salt and substituted argillaceous salt layers for anhydrite layers (Set D). In this calculation, as given in Figure 2, agreement between calculated and measured vertical and horizontal closures is within 2% and 15%, respectively, at 1000 days. The results strongly suggested that the earlier prediction discrepancy has been resolved through use of a better flow potential, a more precise transient creep characterization, the reevaluated material parameters, and an updated stratigraphy. Although the agreement would be slightly modified through the use of the Set A rather than the Set D material parameters and stratigraphy, this would not actually alter the adequacy of the agreement to any significant degree.

Room B is identical to Room D in setting and configuration and gave the same measured response as Room D until onset of Room B heating on day 354, which resulted in a marked increase in observed closure rates. Reevaluated material parameters and updated stratigraphy, except for retaining the 40%

Table 1. Summary of WIPP Structural Test Rooms, Room Complexes, and Shafts

Room(s)	Stratigraphy	Width (m)	Height (m)	Length (m)	Pillar (m)	Remarks
A	salt/arg. salt	5.5	5.5	93.3	18.0	Heated 3 room complex
B	salt/arg. salt	5.5	5.5	93.3	-	Heated overtest
D	salt/arg. salt	5.5	5.5	93.3	-	
G	arg. salt/anhyd.	6.1	3.05	183.9	-	Long room
H	arg. salt/anhyd.	11.0	3.05	round	11.0	Heated round pillar
TRU Pn.	arg. salt/anhyd.	10.1	3.96	91.4	30.5	TRU 4 room test panel
So.Drft	arg. salt/anhyd.	7.6	2.44	1117.0	-	Long south drift
1st Pn.	arg. salt/anhyd.	10.1	3.96	91.4	30.5	First 7 room panel
Q	arg. salt	2.44	diameter	106.8	-	Circular room
CSH Sft	various	3.66	diameter	659.0	-	Construction shaft
AIS Sft	various	6.17	diameter	659.0	-	Air intake shaft

larger argillaceous salt transient creep limit parameter (Set B), was used in the Room B preliminary validation calculation, as given by Munson et al. [7]. This calculation, also shown in Figure 2, was complicated by the heating of the room and provision was necessary to account for heat loss by conduction and infiltration through the doors at the end of the test room. The thermal calculation, while not shown here, was brought into very good agreement by extracting heat along the room periphery. Until day 354, when heating began, the calculated results differ from those for Room D because of the use of different stratigraphies. The heating in the calculation is reflected in an abrupt increase in both vertical and horizontal closure rates. The agreement between measured and calculated vertical and horizontal closures is within 4% and 18%, respectively, at day 1045. We suspect much of the discrepancy in the vertical results is caused by the onset of separation and failures in the roof. Small roof cracks appeared as early as day 650, with definite formation of a thin roof slab starting on day 1045. The continuum creep constitutive model does not treat the localized separation and fracture processes.

Room G is a very long isolated room intended to be "two-dimensional" to exactly match the requirements of two-dimensional numerical solutions. Figure 3 compares the calculated and measured closure results using the Set A reevaluated material parameters and stratigraphy. Although the agreement appears to be very good, the order of the vertical and horizontal closure magnitudes is reversed between calculation and measurement. This result suggests that minor discrepancies can still occur, even though the major prediction discrepancy appears to be resolved. While these minor prediction discrepancies are thought to be well within acceptable uncertainty limits, it may eventually be necessary to resolve some of these minor discrepancies.

A calculation of the South Drift was made using reevaluated parameters and stratigraphy (Set A). Delay (up to 30 days) in gage installation was corrected by reconstructing the missing displacements from the calculated displacements. The "average" of the measured results for ten measurement stations (locations) along the 1117-m-long drift are represented by the measured closures at station 2950, as given in Figure 4. The data from individual stations form a series of essentially parallel curves, with an apparent scatter of ± 10 mm in displacement magnitude at day 1400 caused by an uncertainty of ± 0.5 day in the time between drift excavation and first measurement. Regardless of the measurement uncertainty, the agreement between

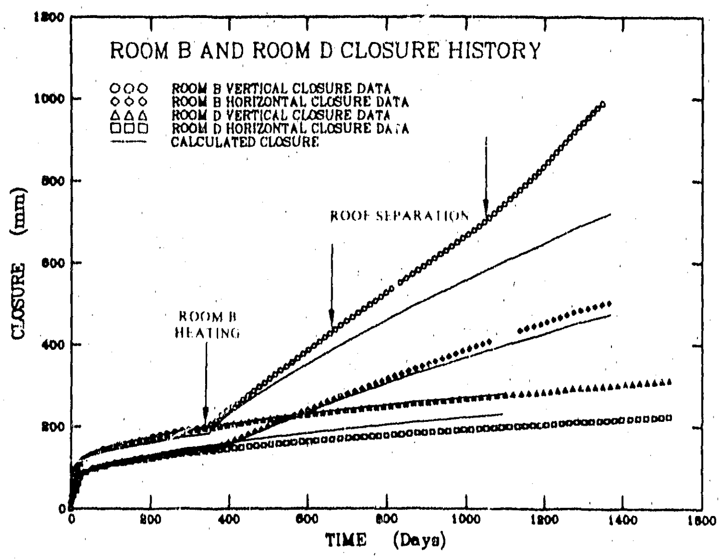

Figure 2 Measured and Calculated Room D and Room B Closures Parameter Set D and Set B, Respectively [after [7])

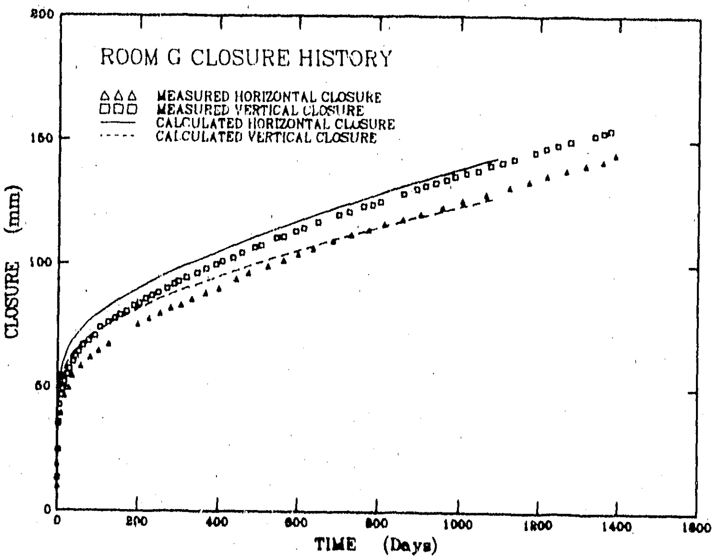

Figure 3 Measured and Calculated Room G Closures, Parameter Set A

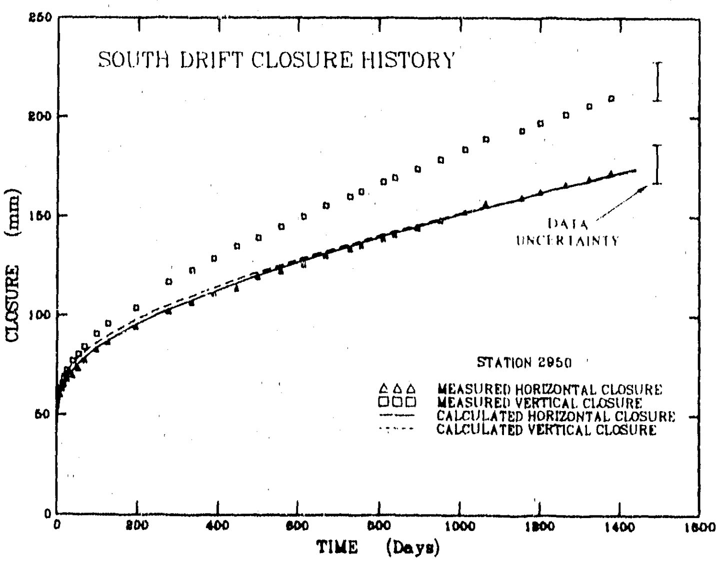

Figure 4 Measured and Calculated South Drift Closures, Parameter Set A

calculation and measurement, as shown in Figure 4, is very good, especially for the horizontal closures where it is well within the known uncertainty of the measurement. The South Drift exhibits the underprediction of vertical closure seen in the Room D, Room B, and (perhaps) Room G comparisons. Because slab separations are observed in both roof and floor of the South Drift, there is a strong possibility that the common discrepancy between calculated and vertical closure is the result of this unaccounted for progressive separation, as is clearly the case for Room B where the separations are quite pronounced.

CONCLUDING REMARKS

Although considerable work remains to be done to demonstrate code validation, preliminary calculations for three isolated rooms of different dimensions and stratigraphic setting, one of which is heated, are quite encouraging. These results suggest the use of a Tresca flow potential, a transient as well as steady-state creep response, the reevaluated material parameters, and an updated stratigraphy is warranted. It remains to be seen if closures of the remaining test rooms and shafts can be successfully calculated, and further, if slab separation effects must be included.

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