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WIPP Room Evolution and Performance Assessment Implications

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"...demonstrations that key aspects of the model and its parameterization are conservative cannot be interpreted to conclude that the present model conservatively predicts the future states of the repository"
Conceptual Model Peer Review Panel (NUREG 1297)

Abstract

Although the Waste Isolation Pilot Plant (WIPP) has demonstrated compliance with the Environmental Protection Agency (EPA) standards, there is an expectation that the project continuously accounts for changes to the technical bases of compliance. The initial performance assessment included twenty four conceptual models that were intended to capture features, events and processes deemed applicable to performance of the repository. Some direct changes occurred within the WIPP framework since the initial compliance certification, such as the requirement for an Option D panel closure system and the types of waste packages actually arriving at the WIPP as compared to the waste modeled for compliance determination. In addition, some of the assumed conditions in the underground setting are demonstrably different than originally modeled, such as the disturbed rock zone. Finally, several unmistakable processes within the room setting are not modeled at all, such as the hydration effects of the magnesium oxide (MgO) engineered barrier and the production of by-products from hydration, corrosion and precipitation. This paper examines five of these elements, the disturbed rock zone, brine availability, MgO, solid production, and room closure, which pertain to the evolution of the WIPP disposal rooms. The initial sections develop the scientific basis supporting an updated view of these five elements with respect to model representations of room evolution. The paper concludes with recommendations for handling each topic as the technical baseline is updated.

1. Introduction

The WIPP performance assessment incorporates features, events and processes into conceptual and numerical models used to predict probable future states of the repository over the regulated period of 10,000 years. Performance assessment, combined with demonstrated knowledge of the disposal system environment, provided justification for EPA's initial certification that WIPP complies with applicable long-term safety requirements.

Uncertainties comprise an important part of the performance assessments because long-term futures are not usually readily predictable. There are two fundamental approaches, probabilistic and deterministic, for dealing with these uncertainties in performance assessment. In probabilistic analyses, such input as scenarios and parameter values are sampled over distributions that are thought to capture the possible range. In deterministic analyses, bounding assessments can be made by selecting conservative parameter values and models, such that the results underestimate the performance capabilities. Both the probabilistic and bounding approaches are implemented in the WIPP performance assessment.

As the knowledge base continues to accumulate from WIPP experience, opportunities to improve the performance assessment modeling become self evident. That is, the performance assessment as currently implemented does not account for existing components of the underground repository (MgO, for example) and continues to represent features, events and processes that are known to be extremely conservative. Parties with an appreciation for the technical baseline for WIPP compliance are aware of many of the inconsistencies residing within the performance assessment models. In many cases, it is assumed that the deviations from reality are conservative because they underestimate the robustness of WIPP. Therefore, if these conservative assumptions still lead to compliance, then there is little perceived harm (and in fact some comfort) in modeling the underground conservatively because its actual performance would be even better than predicted.

The role of Sandia National Laboratories as the science advisor is to provide the best science and engineering information possible to the project. It is therefore a responsibility of the science advisor to continuously appraise progress, to assess the scientific merit, and to utilize this knowledge to provide conceptual models that are as realistic as the available evidence allows. The current representation of the underground evolution as considered for compliance determination deviates significantly from the evolution dictated by the best available information. This paper summarizes a number of ways in which the WIPP room evolution can be more accurately represented.

The remainder of this paper includes a relatively brief overview of several primary elements of the underground setting whose representation can be improved. These sections will discuss both how a feature, event or process is or is not included in the performance assessment model. Each of these sections will conclude with a statement of viability and scientific defensibility of the representation of that particular feature, event or process. After each topic is updated within the technical program, it will be necessary to pose these alternative interpretations to internal and external technical peer review. This paper does not advance the proposition that these concepts must be included in the WIPP performance assessment; that step will involve technical exchange between the DOE and the regulator. Nonetheless, this paper will conclude with a forward view of how these elements might be included in the performance assessment.

2. Features, Events, and Processes Considered

The evolution of the WIPP underground influences several fundamental elements of the performance assessment modeling. The performance assessment models, abstractions and processes have been implemented for regulatory certification of WIPP for the initial compliance certification application (CCA) and subsequent performance assessment verification test (PAVT) in the 1990's and recently for a compliance re-certification application (CRA) which was submitted five years (March 2004) after first receipt of waste (March 1999). Over this period of time, knowledge of the physical, mechanical, chemical, and hydrological setting in the repository has improved because of continued repository science programs and because five years of operational experience allow a more definitive appraisal of various factors involved with disposal of radioactive waste.

Given the experience to date and the fact that the EPA regulations require re-certification at any time or at a minimum of five year intervals, this interim period is an opportune time to re-examine some of the features, events and processes that are included in the performance assessment modeling. In particular, this paper examines actual details of the underground setting--the waste room environment--that are known to exist and are not included in the performance assessment models as well as details that can be modeled more accurately because of advances made in the scientific bases. Performance assessment models can be made more realistic and more accurate by reducing uncertainty with regard to features or processes or by incorporation of known properties of the WIPP waste room that are not included in the current models. By invoking a more representative underground setting, the performance assessment models likewise can be more realistic and uncertainty can be reduced. In addition, a sense of completeness can be obtained if known features of the evolution paths are included in repository analyses while consistency is concomitantly improved if a more complete accounting of the features, events and processes is included in the performance assessment models.

Re-examining and updating the underground evolutionary models can be accomplished by addressing the following questions:

1. What existing elements of the disposal room features, events and processes can be modeled more accurately?
2. What elements of the underground are known to exist and are not included in the performance assessment models?
3. What would comprise the requisite changes to the performance assessment to model waste room evolution more comprehensively and what are the potential impacts to radionuclide releases?

The following list includes elements of the disposal room evolution that will be discussed in this paper:

1. Disturbed rock zone
2. Brine availability to the disposal room
3. MgO hydration
4. Solid production/corrosion
5. Room closure/waste mechanical model

Each element listed above is either not represented in the process models or is included in a manner inconsistent with known facts and observations.

Because performance assessment is the vital link to the EPA's compliance determination, it is imperative that the best possible representation be made of the actual characteristics of the repository. Each of these elements will be discussed in terms of how they are implemented (or not implemented) in the performance assessment and then compared with the actual situation in the repository.

3. Disturbed Rock Zone

The Disturbed Rock Zone (DRZ) constitutes an important geomechanical feature of a WIPP disposal room and is explicitly included in performance assessment. Since the original certification, the scientific understanding of the DRZ has progressed by virtue of ongoing experimental investigations, further evaluations of published research, and international collaborations. The DRZ has been re-examined in considerable detail since operations initiated because DRZ properties are essential to the design and analysis of the panel closure system. The DRZ is an important feature that is included in the performance assessment process models used to predict future repository conditions (e.g., pressure and brine saturation) and brine flow to the accessible environment (e.g., up intrusion boreholes and out surrounding geologic units to the land withdrawal boundary). Furthermore, as modeled, the properties of the DRZ control a significant portion of the brine that can flow into the waste rooms. The most important DRZ properties are the extent (or thickness) of the DRZ, its porosity, and its permeability as they are the three fundamental parameters used for analysis. Basically, the extent of the DRZ as modeled is much larger than will be experienced over the regulatory period and its porosity and permeability will be much lower than modeled as salt fractures in this material heal.

The DRZ implemented in performance assessment extends approximately 12 meters above the roof of disposal rooms and approximately 2 meters below (to the bottom of Marker Bed 139). The porosity of the DRZ used in the performance assessment modeling is defined as being 0.029 greater than the sampled porosity of the undisturbed halite (0.001 to 0.03). The product of the modeled DRZ volume and its porosity is the total amount of brine content in that material that will flow into the waste room if permeability is sufficiently high. Initial performance assessment calculations held DRZ permeability constant at 10^{-15} m^2. Prior to the initial certification determination in 1998, the EPA required a performance assessment verification test, wherein the DRZ permeability was sampled from $10^{-19.4}$ to $10^{-12.5}$ m^2. Actual measurements, observations and experience show that geometry, porosity, and permeability of the DRZ can be more accurately represented.

The WIPP Committee of the National Research Council (NRC) (NRC, 1996, page 4) addressed some of the conservative assumptions relating to the performance assessment models. They noted particularly "The assumption that the DRZ bordering the room excavations remains a relatively high-permeability region throughout the first 10,000 years of the repository appears overly conservative." The NRC committee further states (page 38) "The overburden pressure and deformation will close and heal any fractures that might develop in the disturbed rock zone and seal and isolate any residual gas-filled or brine-filled void spaces in the repository horizon."

Over the period since the initial compliance certification of WIPP, characterization of the DRZ has continued. Hansen (2003) summarizes the contemporary understanding of the DRZ and provides the theoretical and experimental bases for an updated treatment of the DRZ. In essence, the information reviewed by Hansen agrees with the view put forward by the NRC committee and provides technical bases for updating the DRZ conceptual model. The DRZ dimensions and permeability ranges used for the PAVT were not changed for the recent re-certification performance assessment calculations; however, conclusive evidence suggests that the DRZ can be modeled more accurately, which means it would be smaller in extent, and have a lower permeability, thereby limiting the amount of brine that is estimated to flow from the Salado Formation into the disposal rooms.

One of the most important features of salt as an isolation medium is its ability to heal previously damaged areas. Healing arises when the magnitude of the deviatoric stress decreases relative to the applied mean stress. The healing mechanisms include microfracture closure and bonding of fracture surfaces. Microfracture closure is a mechanical response to increased compressive stress applied normal to the fractures, while bonding of fracture surfaces occurs either through crystal plasticity, a relatively slow process, or pressure solution and re-deposition, a relatively rapid process (Spiers et al., 1988). Evidence for healing has been obtained in laboratory experiments, small-scale tests at WIPP and through observations of natural analogs.

It is clear that the DRZ will be very limited in extent over the regulatory period. Hansen (2003) presents the several avenues of scientific approach that lead to this conclusion. Supporting sciences include laboratory testing, theoretical developments, modeling, and observation. Extensive laboratory salt creep data demonstrate that damage can be assessed in terms of volumetric strain and principal stresses. Stress states that create dilation were defined in terms of stress invariants, which allow reasonable models of DRZ evolution and devolution as illustrated in Figure 1. The stress-invariant dilatancy model has been used in structural calculations for more than ten years and remains a viable tool for engineering purposes. Stress-state calculations can be post-processed from numerical analyses to predict disturbed or damaged zones around a typical waste disposal room. The stress-invariant model tracks the stress states such that dilating and healing conditions can be visualized. The salt nearest an opening is expected to undergo the greatest damage and, as a corollary, will also experience the greatest increase in permeability. Salt farther from the opening undergoes much less damage and, as a result, experiences a much smaller change in permeability. Damage is rapidly reversible as shear stresses diminish and mean stress remains essentially constant (Van Sambeek et al., 1993). Healing conditions are created once the salt begins to compress the waste in the rooms.

Salt surrounding the waste rooms will heal by mechanical compression and pressure solution re-precipitation processes and can be considered essentially impermeable ($<10^{-23}$ m^2). The healing processes are extremely fast relative to room closure, occurring in essentially real time. The anhydrite possesses a somewhat higher natural permeability (10^{-19} m^2 to 10^{-21} m^2), which would increase upon fracturing and not be expected to heal as the salt DRZ would. Further, the distorted anhydrite layers (anhydrite "a" and "b"), would tend to deform into the disposal room as the country rock creeps into the opening.

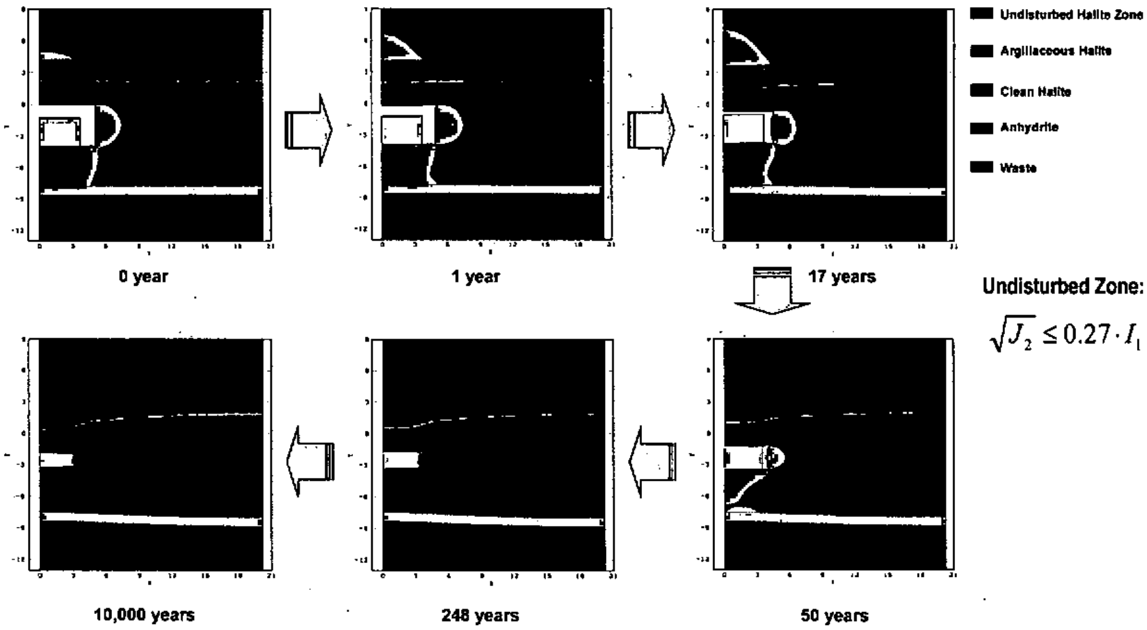

Figure 1. DRZ development and healing around a disposal room (Park and Holland, 2003).

These calculations of the evolution (growth and healing) of the DRZ replicate observations made in the WIPP underground. The predicted size and shape of the DRZ around an opening based on a stress invariant criterion (Figure 1) are similar to the size and shape derived from sonic velocity studies and from microscopy of core damage (Hansen, 2003). The geomechanical model output does not predict permeability directly, but the trend and magnitude of permeability around WIPP openings are understood in considerable detail from field experiments (Beauheim and Roberts, 2002). The modeling in Figure 1 shows how the salt DRZ heals and entombs the waste. Fracture damage in the salt heals as the stresses in the salt approach equilibrium. More details and references of the technical bases supporting these facts are given in Hansen (2003).

4. Brine Availability

Brine is a very important factor in the overall evolution of the repository. Free brine is essential to sustain corrosion of iron and other metals and to possibly promote microbial viability. There is a direct linkage between brine availability and the properties of the DRZ. Although the discussion above concludes that the DRZ will be limited in extent and heal to a state approaching in situ permeability, the conceptual model implemented in performance assessment represents something quite different. The performance assessment modeling will be compared to field observations of brine sources and brine flow in the discussion below.

The BRAGFLO model used for calculating brine and gas flow within and surrounding the repository includes a large zone of DRZ (extending 12 m above the room and 2 m below) for which a single permeability value is sampled and held constant for 10,000 years. The pore volume of this material is initially assumed to be completely filled with brine. The head gradient between the far field and the room initially is very high (difference between lithostatic and atmospheric pressure) but decreases with time as an increasing amount of gas is generated. The performance assessment models initiate gas generation immediately, which would not occur unless free brine was available. If permeability is high enough to allow brine flow under these conditions, nearly all the brine contained in the DRZ can flow into the waste rooms. In order to account for brine loss due to mine ventilation during the operational period, all brine flowing into the waste rooms during the first five years is removed from the model. After this relatively brief time, it is assumed that ventilation will have ceased (panel closures have been emplaced). Typically, only a small amount of total available brine in the DRZ flows into the waste rooms during this five-year period. By far, most of the brine in the DRZ is still available to flow into the waste rooms after this operational period, especially if a high DRZ permeability was sampled.

Beauheim and Roberts (2002) performed an evaluation of Salado Formation hydrology and hydraulic properties. They conclude that "*On the time scale of the operational period of WIPP (decades), the far field lacks the capacity to fill all of the newly created porosity in and around the repository, much less pressurize it to near lithostatic pressure. After WIPP is closed, far-field flow toward the repository will continue, but the overall "healing" of the formation around the repository (closure) and compaction of the crushed-salt backfill will act to reduce both the hydraulic gradient and the porosity present near the waste. Thus, the amount of brine that ever comes into contact with waste will be controlled by the relative rates at which brine flow and repository closure occur.*" It is noted that no crushed salt backfill is emplaced in the disposal rooms, but the fundamental conclusion of limited brine inflow remains.

The porosity in the rocks surrounding WIPP is very low, on the order of 0.01. Because salt is a creeping medium, the pore pressures within the pores is expected to be near lithostatic. Although the natural geologic materials in which WIPP is located possess very low permeability, some variation exists between anhydrite, clay and salt layers. The lateral permeability of clay and anhydrite is higher than undamaged salt, which is essentially impermeable. Anhydrite permeability derives from naturally occurring bedding-plane fractures (Borns, 1985). Beauheim and Roberts (2002) conclude that flow through the Salado Formation is horizontal, parallel to bedding.

An extensive brine sampling and evaluation study was conducted in the WIPP underground for over a decade (Deal et al., 1995). Soon after mining, moist areas were noticed by geotechnical personnel and it was apparent that not all brine was bound to hydrous minerals or sealed inside fluid inclusions. The clear salt contains the least water by weight (0.3%), argillaceous salt contains somewhat more (1.5%) and clay by itself contains the most (>2.2%), according to Deal et al. (1995). The brine sampling and evaluation program (BSEP) adopted a mission to investigate the origin, hydraulic characteristics, extent and chemical composition of brine in the Salado Formation at the repository horizon and the seepage of that brine into excavations at the WIPP. The BSEP program noted that after 11 years of study brine is remarkably hard to find in the WIPP excavations.

Based on the actual conditions and observations summarized above, it is clear that the DRZ has essentially dewatered in the period between mining and waste disposal. As the extent of the DRZ diminishes as a result of healing and the corresponding permeability decreases, any remaining brine in the DRZ will become trapped. Room closure characteristics promote salt DRZ healing and fluid flow is dominantly horizontal. To quantify these generalities, Beauheim and Roberts (2002) offer this for context: *"To whatever extent regional flow is occurring under the naturally occurring gradients, it is expected to be toward areas of lower overburden pressure. Flow is expected to be unmeasurably slow, however. Given a halite permeability that we think might be representative of far-field conditions of 10^{-22} to 10^{-21} m^2 (hydraulic conductivity of ~10^{-15} to 10^{-14} m/s), a hydraulic gradient of 0.01, and a porosity of 0.01, brine would take between 3 and 30 million years to flow one meter. In anhydrite, where the permeability might be one hundred times higher, brine would still take 30,000 to 300,000 years to flow one meter."* Therefore, brine from the Salado Formation would be prevented from entering the disposal rooms in normal undisturbed conditions. A "dry repository" constituted one of the perceived attributes when Salado Formation salt was identified as a strong candidate for nuclear waste disposal.

Brine available to the repository horizon will be extremely limited by the nature of the DRZ but in addition, any brine that does enter the repository will immediately react with the abundant magnesium oxide (MgO) chemical barrier and be prevented from reacting with the waste and containers. The NRC (1996, page 5) concluded that "*Gas generation will be minimal in a dry or nearly dry repository such as WIPP because both chemical and biological gas generating processes (e.g., metal corrosion and bacterial action on organic matter) require a liquid phase for mass transport of the reactants and products that are involved in gas formation.*" The findings of the NRC WIPP committee were issued essentially at the same time performance assessment calculations were completed for the initial compliance determination. At that time, the performance assessment process models included 12 m of high permeability DRZ and instantaneous gas generation, but did not include the presence of MgO. These representations and omissions were thought to present a "conservative" performance assessment, despite a stark inconsistency with known facts.

5. MgO Hydration

At the rate of current operations, nearly 70,000,000 kg of MgO will be placed in the ten waste panels. The regulatory requirements and technical reasons for placing MgO are to ensure a pH that minimizes actinide solubility, as will be discussed in more detail later in this section. Although MgO is placed in vast quantities throughout the waste rooms, its hydration characteristics are not included in the performance assessment models. If the evident hydration attributes of MgO are considered, a mechanism for brine consumption exists. There is sufficient MgO to consume all the natural brine available from the WIPP horizon prior to the occurrence of an inadvertent human intrusion. This actuality further assures that the waste disposal areas will be dry.

Gas-producing processes in the WIPP have been postulated for conditions in which brine is available for reaction. These include anoxic corrosion of Fe- and Al-base metals that produces hydrogen, consumes the brine water, and precipitates the dissolved salts. Further, possible anaerobic microbial degradation of cellulosics and, perhaps, plastics and rubbers could produce methane, carbon dioxide, hydrogen sulfide and nitrogen (CH_4, CO_2, H_2S, N_2). Owing to the uncertainty assumed for these processes, a decision was made for the CCA performance assessment to allow microbial gas generation in only half of the performance assessment realizations. In one half of these "microbial" realizations (25% of the total realizations), microbes were assumed to consume only cellulosics. In the other half, microbes were assumed to consume all the organic materials. More recently, during EPA's completeness determination for the first recertification, it appears that EPA may require a change the conceptual model for microbial gas generation. There are two main changes under consideration by EPA: (1) microbial degradation of cellulosics is assumed in 100% of realizations (still 25% of realizations will include the degradation of plastics and rubbers), and (2) the inundated and humid rates of microbial degradation are to be significantly reduced based on results from nearly ten years of gas generation experiments done at Brookhaven National Laboratory. The final BRAGFLO runs incorporating these changes have yet to be finished and therefore all BRAGFLO results used in this report are from the CRA calculations using the CCA/PAVT microbial gas generation parameters. These reactions require brine or water vapor to be present, but the consumption of water is assumed to have no net effect on the water content in the repository.

The MgO was added as an engineered barrier for the primary purpose of sequestering CO_2, and thus controlling the pH and decreasing solubility of actinide elements in brines. The original compliance certification application asserted that MgO, panel closures, shaft seals, and borehole plugs would satisfy the EPA's assurance requirement for multiple natural and engineered barriers because they meet the definition of barriers as "*any material or structure that prevents or substantially delays movement of water or radionuclides toward the accessible environment*". However, EPA ruled in its May 1998 certification of the WIPP that MgO is the only engineered barrier, and approved emplacement of approximately 70,000 tonnes in the repository. The MgO would decrease actinide solubilities because it will remove carbon dioxide and maintain the brine pH within a favorable range. The function of MgO is predicated on the presence of brine. Ongoing lab studies demonstrate that MgO hydrates and consumes water, thus contributing to the assurance that the WIPP will remain dry.

The concept behind the MgO engineered barrier is that it will govern chemical conditions in the repository and control radionuclide solubilities, and thereby substantially reduce the potential for transport of radionuclides. The MgO is an assurance measure that is placed in sufficient quantity to consume all CO_2 that could be produced by microbial consumption of the cellulosics, plastics and rubber in the waste. These aspects of the MgO effect are implemented in performance assessment by assigning a range to actinide solubility in the brine. Underlying this process model are assumptions that the repository rooms have ample liquid brine available and that the waste is readily soluble. Although considerable detail of actinide solubility has been incorporated in performance assessment models, the process models do not account for the hydration reactions between brine and MgO.

Supersacks containing MgO are arranged on top of every waste stack as shown in the photograph in Figure 2 of waste placed in Panel 1. At the rate of current operations, nearly 70,000,000 kg of MgO will be placed in the ten waste panels. On an area basis, this equates to nearly 475 kg/m^2. Roof-to-floor closure will bring the superincumbent salt onto the MgO supersacks in approximately 10-15 years. As the salt compresses the waste stack, breakage of the supersacks would cascade granular MgO into the interstitial void space between waste columns. It is possible that minor amounts of roof salt will disaggregate and fall into the interstices, as well, but disposal room roofs are latticed with rock-bolted chain link, which would minimize collapse of the roof beam. Following this logical reasoning, available floor space will be littered with granular MgO at an early stage of WIPP room evolution.

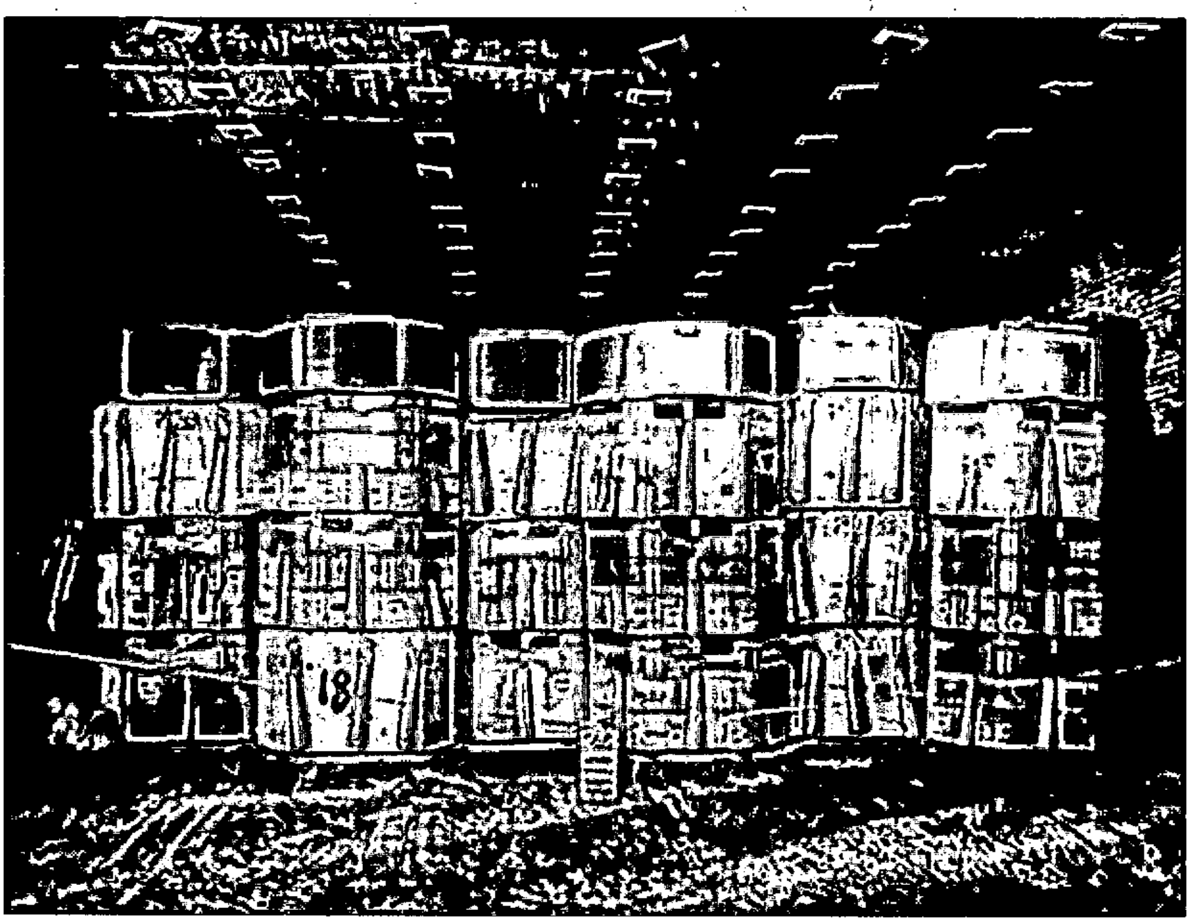

Figure 2. Waste and Magnesium Oxide Placement in a WIPP Disposal Room

The "dryness" of the repository is assured because—from arguments above—there is very limited brine available to the repository room in the first place. Previous sections assert that a healed DRZ presents a low permeability barrier to the ingress of brine from the Salado Formation and that an extensive brine sampling program shows that there is little brine available to the underground. The DRZ permeability is very low because of healing, such that only small volumes of rock with accessible brine lie in close proximity to the disposal room. Thus, the MgO would consume the small volume of brine that might enter the room from the DRZ.

These arguments logically suggest that a more thorough conceptual model for the WIPP performance assessment can be developed to incorporate MgO hydration and more realistic hydrologic properties for the DRZ (Hansen, 2003). When and if the hydration reaction between MgO and brine is acknowledged by including these reactions in the process models, it is a necessary condition that any brine present will be consumed by the hydration reaction. Owing to the presence of MgO alone—and with no other factor—the repository room must stay dry until such time as human activity introduces abundant additional brine from a reservoir, such as in the underlying Castile Formation or the overlying Culebra.

If the arguments put forward above for DRZ healing and minimal brine availablility are ignored, and the DRZ model is left unchanged from that which exists in the current performance assessment, the MgO hydration would <u>still</u> have a profound drying effect on the repository rooms. Here is an example of why this is so.

Gas generation, whether by corrosion or by microbial consumption of cellulosics, plastics and rubbers, requires brine. ***If*** brine infiltrates the room, it is expected to first react with the MgO to form $Mg(OH)_2$ (brucite). This reaction involves consumption of brine and an increase in volume of the former MgO granules. In addition, brine consumption gives rise to precipitation of NaCl and other dissolved salts, which also leads to a lowering of room porosity. Using the current performance assessment models, the following calculation of brine inflow and consumption by hydration shows that even for realizations producing the maximal amounts of brine into a waste room, there is more than sufficient MgO to consume that brine by hydration.

1. Assume 67,132,800 kg of MgO to be emplaced in 10 panels.
2. Assume 90% of aggregate MgO is pure periclase (60,419,520 kg)
3. Equal to 474.77 kg/m^2.
4. It would take 21 cm/m^2 of water in the CH-waste-filled repository to fully hydrate the periclase to brucite.
5. Pre-hydrated MgO solids volume (assuming periclase density) accounts for 14 cm/m^2 of CH-waste-filled repository.
6. Full solids volume of hydrated brucite accounts for 29 cm/m^2 of waste-filled repository (~100% volume increase). The volume increase would be greater if the precipitation of the dissolved salts in the brine were also included.
7. CRA R1 S1 had a maximum brine inflow equal to 22 cm/m^2 of waste-filled repository in the first 100 years (max of 39 cm/m^2 of waste-filled repository for 10,000 years).

If we assume that a given brine volume is equal to volume of pure H_2O in that brine, then in nearly all vectors of the undisturbed scenario, hydration consumes all brine in the first 100 years. Thus, even with the overly large DRZ used for the CCA and CRA modeling , at 10,000 years there are 8 vectors that have more brine entering than can be consumed by hydration of MgO. If the DRZ were treated appropriately and the estimation of the amount of brine limited to the reasonable maximums available, there exists sufficient MgO to hydrate all available brine.

This calculation shows that even when the current representations of the DRZ and brine inflow are evaluated, there is sufficient MgO such that the presence of liquid brine in the repository is very unlikely, especially at early time, when the DRZ permeability is sufficiently high to allow brine to flow into the rooms. Evidence provided above demonstrates realistically that volumes of brine available to the underground would be severely limited. Thus, the undisturbed repository will not have free brine necessary for gas generation.

Another point to be made with respect to brine available to the underground disposal rooms concerns possible lateral movement of brine, should it exist. Implementation of the Option D panel-closure system in performance assessment has eliminated lateral migration of brine from the waste-free areas in the WIPP underground workings to the waste-filled areas (Hansen et al., 2002; Stein and Zelinski, 2003). The inclusion of the Option D panel closures has decreased the estimated brine saturation of the waste, at least during the period of undisturbed conditions prior to human intrusion. This decrease in saturation decreases the probability of significant microbial activity prior to human intrusion, and decreases the probability of survival of microbes thereafter as well.

6. Solids Production/Corrosion

The conceptual model of gas production in the WIPP disposal room includes approximately equal contributions from microbial degradation, which is considered to be uncertain, and metal corrosion, which is assumed to occur in every realization. The current model for metal corrosion <u>does</u> account for water consumption and an example is given here. Using results from performance assessment calculations, the water consumed by corrosion in the undisturbed scenario of the CRA R1 at 100, 1000 and 10000 years is calculated by assuming the following reaction:

$$Fe + 2H_2O \rightleftharpoons Fe(OH)_2 + H_2.$$

This reaction acts on iron surfaces at a sampled rate (0 to 3.17×10^{-14} m/s) consuming two moles of water for every mole of iron corroded. The products are assumed to have the composition $Fe(OH)_2$ and hydrogen. Here are the area normalized results [m^3 of water consumed /m^2 waste filled repository] for the CRA, Replicate 1, undisturbed scenario (R1 S1):

Water consumed per square meter in the CRA R1 S1

Time [yrs]	Minimum	Median	Maximum
100	0 cm	0 cm	2 cm
1,000	0 cm	4 cm	12 cm
10,000	0 cm	7 cm	23 cm

Thus, at most, corrosion consumes about the same amount of water that would be consumed by MgO hydration. Based on excursion runs with greater Fe surface area per volume of waste, faster corrosion reactions actually dry the repository and result in fewer vectors consuming all the biodegradable material. This is a strong indication that if performance assessment incorporated MgO hydration, the prediction of microbial degradation would be essentially indefensible.

The corrosion of iron also results in an increase in solids volume. For every cubic meter of iron corroded the volume of the resulting corrosion products is over 4 m^3. Using results from the CRA R1 S1, this volume increase accounts for between 2 and 14 cm of additional solids volume per square meter of repository.

It has been noted previously that brine consumption also precipitates the dissolved salt. The formation of these precipitates would have the effect of reducing waste room porosity over and above the reduction predicted from creep closure and waste compaction. In addition, these crystallites would have a further effect of suturing surfaces and producing a cohesive architecture within the waste. As a first approximation of the volume of salt precipitated per cubic meter of brine, one can determine the difference in brine and water density (1220 kg/m^3 – 1000 kg/m^3) = 220 kg salt/m^3 brine. Given halite density of 2170 kg/m^3 the volume of precipitated salt is approximately 0.1 m^3 halite/ m^3 brine. Therefore, 10% of the brine consumed either by corrosion or though MgO hydration would be precipitated as salt crystals.

A rough estimate of the combined impact on room porosity of precipitation of salts and the volume increases due to hydration and corrosion reactions is presented next. It is expected that within the first 100 years of performance, most of the creep closure will have occurred and the height of the waste-filled rooms will have gone from an initial 4 m to approximately 1.5 m. As a result of this closure, the room porosity is estimated to have reduced from an initial value of 0.85 to a value near 0.25. A porosity of 0.25 in a room with a height of 1.5 m is the equivalent of 37.5 cm of open pore space per square meter of repository. Examining results from the CRA R1 S1, the total amount of potential volume increase due to MgO hydration ranges from 0 to 15 cm per square meter of repository. The total amount of potential volume increase resulting from corrosion ranges from 0 to 14 cm per square meter of repository. It is clear from these results that even if the DRZ is represented as a thick region with high permeability, the potential magnitude of the solids volume increase could significantly plug up nearly all the available porosity in the rooms.

These conditions are suggestive, but cautious interpretation is in order because this system is highly coupled and perhaps self limiting. For example if porosity changes were included in the modeling, the amount of brine that enters the waste rooms would likely be significantly reduced as would the permeability of the waste rooms. If changes to the DRZ permeability, porosity and extent were also included, it is very likely that brine inflow and significant gas generation would cease to dominate the performance assessment results.

7. Room Closure/Waste Mechanical Model

The evolution of the underground setting involves many features, events and processes, which are vital to performance assessment. One technique employed for performance assessment involves coupling between mechanical closure of the waste room and the multiphase flow code, BRAGFLO. The waste room evolution is evaluated in terms of a porosity surface, which embodies salt creep, mechanical deformation of the waste and gas generation. These data are sampled during execution of the BRAGFLO code. Additional realism to the conceptual models and inclusion of known phenomena can improve the technical bases for room evolution and implementation of the performance assessment calculations.

The porosity surface implementation in performance assessment for the CCA and CRA uses a volumetric plasticity model that was developed from laboratory tests on 55-gallon drums of simulated waste. The model does not account for the physical/mechanical effects that chemical/microbial degradation imparts on the waste room inventory. It should also be noted that the waste packages already disposed include several forms other than 55-gallon drums. Obviously, massive changes to the waste packages caused by corrosion and microbial consumption would affect room closure and porosity surface development and massive changes to the waste <u>are necessary</u> to create gas pressure.

The porosity surfaces created for the original certification and those created subsequently for other possible waste packages, did not and do not include the structural effects of degradation, nor do they include structural effects of MgO hydration, salt precipitation, and corrosion by-products. All of these processes would occur if a significant amount of brine enters the waste room and the hypothetical gas generation scenarios ensue in the WIPP underground. The manner in which room closure is considered in the performance assessment today is based on two contradictory future states of the waste: one of degradation to produce gas and another of intact 55-gallon drums for room closure calculations. As it turns out in these analyses, when any significant gas is generated the mechanical response of the waste has little to do with room closure because the gas holds the room open and waste compression ceases.

As presented in detail in the first part of this paper, the future state of the disposal rooms are unlikely to contain free water until brine is introduced by a drilling intrusion into a Castile brine reservoir. Given the current drilling rates, the average time to the first drilling intrusion is approximately 1000 years. Because of institutional controls, it is assumed in performance assessment that no drilling will occur for at least 100 years because of institutional control of the site. It has been shown that brine availability is limited and that processes of MgO hydration and (possibly) metal corrosion would consume far more brine than could be produced in the undisturbed setting, especially in the first 100 years. A proper model for room closure would involve compaction of waste, hydration of MgO, and precipitation of salt in proportion to the volume of brine consumed. Recommendations regarding how to model the room closure processes are made in the next section.

8. Recommendations

The goal of this review of repository characteristics is to reduce uncertainty by improving process models used in performance assessment and to include features, events and processes that are known to exist and are not currently incorporated in the performance assessment. This section identifies a proposed plan forward for implementation of these elements in PA. More specifically, any modifications suggested toward the stated goal would involve code modifications to BRAGFLO version 5.0 to incorporate a more current and sophisticated understanding of the underground environment and many of the important processes at the WIPP. The purpose of these recommendations is to introduce the issues into a technical review forum, first by identifying the potential issues and then by providing possible approaches to address them. If these changes are brought forward for consideration by the EPA, they will first necessitate a conceptual model peer review.

8.1 Disturbed Rock Zone

Issue:
Currently the extent of the DRZ is fixed and permeability is sampled. The DRZ is not allowed to heal over time, which is completely unrealistic. Healing will affect porosity, permeability, and the geometry of the DRZ. The current model for the DRZ also provides the source for brine, such that improving the DRZ model would also address the issue of brine availability until the first intrusion.

Recommendation:
Based on arguments summarized by Hansen (2003), the evolution and devolution of the DRZ is known with considerable certainty. The proposal would be to use the stress invariant damage criterion (I_1- J_2 from Van Sambeek et al., 1993) to quantify the maximal extent of the DRZ. Based on a geometric approximation from structural calculations, we would allow the brine from this zone to access the disposal room. This brine would then be reacted with MgO and we could take a look at by-product solids produced and what conditions this hydration might impart to the waste architecture.

8.2 Brine Availability

Issue:
The recommendations for proper treatment of the DRZ would also ensure consistency with limiting brine availability. There are additional elements of the underground setting that are pertinent to brine availability. One factor currently implemented in the performance assessment is called "waste wicking" and another issue pertains to room closure "humid" environment.

The modeling assumption of waste wicking would require modification to achieve consistency. Gas generation rates used by BRAGFLO should be proportional to the brine saturation in each of the computational cells representing the waste areas in the BRAGFLO grid. However, in an attempt to account for the possibility that liquid brine could be available to waste material in the upper part of the waste stacks by way of wicking, this proportionality is not maintained. As a result, vectors with very low brine saturations can have gas generation rates that would be expected for a much wetter repository. The problem is in the way performance assessment implements the wicking process in BRAGFLO. Currently BRAGFLO implements wicking in the waste by sampling a random variable (WAS_AREA:SAT_WICK) from a uniform distribution from 0 to 1. This random value is then added to the value of brine saturation calculated by BRAGFLO in each cell to yield a quantity referred to as the "effective saturation". This effective saturation is used to determine the gas generation rates used in BRAGFLO. The effect of this implementation is that for many vectors the effective saturation value is dominated by the sampled wicking value rather than the true brine saturation and thus gas generation rates tend to be much higher than would be predicted. This issue was not as important during the CCA and PAVT because brine saturations in the waste predicted by BRAGFLO were relatively high in many vectors. However, due to the Option D panel closures, the brine saturation in the waste areas is predicted to be much lower in the CRA than for the CCA and PAVT. Because the current implementation adds the random wicking variable to the brine saturation, it causes very low brine saturation conditions to produce gas at relatively high rates, when such rates could not possibly be sustained given that there is so little brine available.

It is possible that in the first 100 years some brine drains downward along preferentially oriented fractures. As noted by the NRC (1996) this brine would gravitate to the anhydrite marker bed below the repository horizon (MB 139). This possible scenario prevents the brine from reaching either the MgO or the waste packages. However, it does create a "brine humid" environment, which may initiate MgO hydration and may increase the creep rate. High relative humidity enhances creep deformation of salt, so a brine humid environment may have a first-order influence on room closure.

Recommendation:
This issue needs to be studied and a solution implemented that ensures that the wicking process redistributes brine that is already in the room rather than add brine for the purpose of calculating gas generation rates. This change is related to implementation within the code and pertains to treatment of the available brine in a more appropriate manner.

8.3 MgO Hydration

Issue:
Performance assessment must account for MgO in the underground setting. The initial impact of MgO is brine consumption.

Recommendation:
The first step is to establish the fact that MgO would preferentially consume brine before corrosion. Currently BRAGFLO includes the process of brine consumption in the corrosion reaction. Hydration of MgO was considered for addition to performance assessment previously, but subsequently removed due to QA considerations. A review of

this past work is needed and a decision made on the viability and defensibility of including MgO hydration in the next version of BRAGFLO.

8.4 Solids Production/Corrosion

Issue:
Currently the only significant mechanism that allows the porosity of the waste regions to reduce over time is creep closure, implemented in the porosity surface. There are other processes that will affect waste room porosity that should be included into the model.

a. The transition from MgO to brucite is accompanied by an increase in the volume of the solids.
b. The corrosion of iron results in an increase in the volume of the solids
c. All brine consumption will lead to precipitation of dissolved solids in the brine leading to an increase in the volume of the solids.

Recommendation:
It may be most realistic to model room closure and porosity decrease over for a period of time, say 100 years. The void space reduction from creep closure will be further decreased by solids production from the processes listed above. Then a new condition of the underground setting could be implemented (essentially start the performance assessment under these new conditions). At some future date, drilling can be modeled to inundate this new room setting.

8.5 Room Closure Model/New Conditions at t > 100 years

Issue:
The other issues identified above give rise to a new look at what performance assessment needs to capture. Technical issues strongly advocate for a dry repository until such time that an external source of brine may inundate a waste panel. So the issue is: what does the waste room look like at that future date?

In addition, the room closure model as implemented in performance assessment is highly dependent on gas generation. Currently BRAGFLO is able to implement only a zeroth-order gas generation reaction. It would be useful to allow variations in the kinetic models in order that the results of long-term gas generation experiments could be implemented directly into the BRAGFLO model. Consultation with the geochemistry group will be required to guide this change.

Recommendation:
Resolution of room closure issues depends in part on how we reconcile the other issues, but some things are clear. The first proposition is that the room remains dry until a future drilling event introduces brine. Little gas is generated under the undisturbed scenario until after an intrusion because of the overriding effect of MgO hydration and possible consumption of brine by metal corrosion processes. The waste will have been compacted in a dry environment. When the new source of brine inundates the room, it may fill all

the available interstitial space. So, we need to hydrate the remaining MgO and begin corrosion, while simultaneously depositing the new solids and salt precipitate.

When the first panel is flooded it will almost immediately be in a near lithostatic condition. The interstitial pore space will be filled with incompressible fluid. Panel closures are effective at isolating a flooded panel from the rest of the repository until pressures exceed lithostatic and fracturing can occur. The introduction of brine from the intrusion will start gas generation processes and pressures would increase. If the panel has had 100 years or more to consolidate, presumably there will not be all that much pore space for brine to fill and further hydration and corrosion may effectively plug much of the remaining pore space after the intrusion. If gas generation proceeds enough to open up fractures between panels, this could lead to the transport of additional brine to the repository and into other panels.

The impact of the porosity surface on performance assessment was evaluated by Hansen et al. (2004). Their analysis shows that repository conditions are not greatly affected by the uncertainty in waste structural properties and spatial arrangement, as characterized by the uncertainty in the porosity surface. Moreover, the total releases at probabilities above 0.001 are relatively unchanged by the use of different porosity surfaces. Thus, the uncertainty in waste structural properties and spatial arrangement, as represented by the uncertain **porosity surfaces, is not significant in the performance assessment**. They concluded that a single porosity surface is appropriate for performance assessment.

As the WIPP program moves forward, it is essential to continuously evaluate the bases for demonstrating performance certification. When the conditions in the underground change or new and better information become available, it is an inherent responsibility to adjust to these new circumstances to the limit that the knowledge allows. When the current features, events and processes are examined, many clear differences emerge between what is known and what is modeled. Incorporation of updated conditions will reduce uncertainty, account for actual conditions, and provide a more realistic and robust repository than currently modeled for performance assessment.

Milestone Completion: This paper meets the stated objective of Milestone 3/15/2005 in Rock Mechanics "Complete a position paper detailing a realistic evolution of the WIPP underground. This paper will review elements of the repository that are currently not included in performance assessment (such as MgO) as well as elements that are included in the performance assessment but can be improved upon based on advancements in our technical understanding (such as the DRZ) and include a proposed plan for implementation of these elements in future analyses.

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