# Title 40 CFR Part 191
# Compliance Certification
# Application
# for the
# Waste Isolation Pilot Plant

## MON Attachment 1

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# CONTENTS

# TABLES

# ACRONYMS

| | |
|---|---|
| CCDF | complementary cumulative distribution function |
| CFR | Code of Federal Regulations |
| DOE | U.S. Department of Energy |
| DRZ | disturbed rock zone |
| FEPs | features, events, and processes |
| LHS | Latin hypercube sampling |
| WIPP | Waste Isolation Pilot Plant |

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# MONPAR

## MONPAR.1 Analysis Methodology

In accordance with 40 Code of Federal Regulations (CFR) § 194.42(a), the DOE has analyzed the effects of disposal system parameters on the containment of waste in the disposal system. The results of the analysis are to be used in developing plans for preclosure (operational) and postclosure monitoring. According to 40 CFR § 194.42(c), the objective of the analysis is to identify parameters that are significant. The analysis included the items described in 40 CFR § 194.42(a):

> (1) Properties of backfilled material, including porosity, permeability, and degree of compaction and reconsolidation;
>
> (2) Stresses and extent of deformation of the surrounding roof, walls, and floor of the waste disposal room;
>
> (3) Initiation or displacement of major brittle deformation features in the roof or surrounding rock;
>
> (4) Ground water flow and other effects of human intrusion in the vicinity of the disposal system;
>
> (5) Brine quantity, flux, composition, and spatial distribution;
>
> (6) Gas quantity and composition; and
>
> (7) Temperature distribution.

Significant parameters are defined in 40 CFR § 194.42(c) as those that "affect the system's ability to contain waste or the ability to verify predictions about the future performance of the disposal system."

In this analysis, the U.S. Department of Energy (DOE) has used an approach which is consistent with previous work regarding disposal system performance, and is also consistent with the criteria for certification, as described in this appendix.

The term parameter is used in 40 CFR Part 194 to describe properties and processes in the disposal system. While this use is somewhat inconsistent with the DOE's use of parameters in the mathematical modeling system, the DOE has considered parameters, properties, and processes in this analysis to satisfy the criteria of 40 CFR § 194.42.

40 CFR § 194.42(c) says "A disposal system parameter shall be considered significant if it affects the system's ability to contain waste or the ability to verify predictions about the future performance of the disposal system." The DOE has implemented these criteria for significance in this analysis as follows:

- A parameter's effect on "the system's ability to contain waste" has been evaluated in terms of its potential effect on compliance with the regulatory release limits.

- A parameter's effect on "the ability to verify predictions about the performance of the disposal system" has been evaluated in terms of verifying the assumptions used in modeling the system's performance.

The waste containment requirements in 40 CFR § 191.13 are defined as compliance with the release limits in 40 CFR § 191.13(a) and with the individual and groundwater protection standards in 40 CFR § 191.15 and 40 CFR § 191.24, respectively. Containment and compliance are directly related: properties and processes which are significant for waste containment are also significant for compliance with the release limits. Therefore, the DOE uses compliance with the release limits as the performance measure to determine which parameters are significant to waste containment.

The DOE may verify assumptions used in system performance in one or more of the following ways:

- Measurement of physical and chemical conditions to see if they remain consistent with expected conditions or within the range of conditions incorporated into the assumptions and models. This is useful only for those conditions that are significant to calculated system performance.

- Measurement of physical and chemical processes that are currently modeled based on professional judgement or regulatory guidance because data are not available. This may be applicable to processes that are significant to system performance and have not been considered in previous performance assessments.

As described in Section 6.4.11, the parameter database includes the parameters used in performance assessment codes. The parameters in the database fall into two broad categories: those that are assigned fixed values, and those that are uncertain and are therefore assigned a range of values.

The DOE considered the major processes and models described in Section 6.4 and the results of previous performance assessments and developed an initial list of potentially significant parameters to be subjected to this analysis. Parameters were included in this analysis because they met one or more of the following criteria:

- The parameter represents one or more important aspects of the process or model

- The parameter represents subjective uncertainty (such as spatial variability in a physical property or process used in modeling results of repository performance)

- The parameter represents stochastic uncertainty (such as drilling rate for consideration of human intrusions)

- The parameter represented subjective or stochastic uncertainty in previous preliminary performance assessment calculations (such as the diameter of the drill bit in the intrusion borehole)

- The parameter proved to be moderately to highly sensitive in previous preliminary performance assessment calculations (for example, 1991, 1992)

The DOE assigned a range of values to each of the uncertain parameters used in the performance assessment. The subjective parameters are the basis for creating the vectors (sets) of parameter values using Latin hypercube sampling (LHS) in the Monte Carlo analysis described in Section 6.1.5. The stochastic parameters that represent the probability of plausible and important events are subjected to random sampling in construction of the complementary cumulative distribution function (CCDF) used in comparisons with the release limits in 40 CFR § 191.13(a).

In the analysis of parameters discussed in this appendix, the DOE considered the parameters meeting the criteria listed above, together with the properties and processes identified in 40 CFR § 194.42(a). Each parameter is considered in the context of scenarios where it may be significant. As described in Section 6.2 and Appendix SCR, there are three categories of features, events, and processes (FEPs) that are screened for scenario construction:

- Natural FEPs

- Waste- and repository-induced FEPs

- Human-initiated events and processes

The results of the analysis of the effects of disposal system parameters on waste containment are organized into the same three categories and are presented in the following sections.

## MONPAR.2 Potentially Significant Parameters for Describing Natural Properties and Processes

The parameters for describing natural properties and processes that were considered in this analysis fall into seven groups:

- Hydrologic properties of the undisturbed Salado Formation, including properties that govern brine quantity, flux, and spatial distribution.

- Composition of brine in the Salado.

- Hydrologic properties of the undisturbed Culebra Member of the Rustler Formation, including properties that govern brine quantity, flux, and spatial distribution.

- Composition of brine in the Culebra.

- Hydrologic properties of the undisturbed Castile Formation, including properties that govern brine quantity, flux, and spatial distribution.

- Composition of brine in the Castile.

- Natural temperature distribution in the disposal system.

The results of the DOE's analysis are presented in Table MONPAR-1. The parameters describing natural properties and processes are discussed in the following section.

### *MONPAR.2.1 Salado Hydrology*

*Hydrologic properties of the intact Salado Formation are incorporated into performance assessment through use of parameters which are consistent with extensive experimental observations.*

*Variations in these parameters have a moderate effect on system performance assessment. There is no indication that properties of the intact (far-field) Salado will change during the regulatory period; thus they will not be monitored during the operational period nor during the postclosure period.*

The Salado is made up of low-permeability beds of variable composition. The low permeability provides a hydrologic barrier in all directions between the repository and the accessible environment. The structure of the Salado and its bedded hydrostratigraphic units are incorporated into the geometry of the performance assessment models as discrete regions (Section 6.4.2). The Salado in the vicinity of the repository is composed mainly of pure and impure halite and anhydrite. A large amount of information about the hydraulic properties of these materials has been collected through field and laboratory experiments.

Excavation of the repository has altered natural pressure gradients in the Salado, creating the potential for fluid flow. The properties of the rock in the zone surrounding the repository have also been altered in response to the pressure gradients. This disturbed rock zone (DRZ) and its properties are discussed in Sections MONPAR.3.1, MONPAR.3.2, and MONPAR.3.3.

In the intact Salado (outside the DRZ), hydrologic parameters for the layers are uniform and constant, with the exception of porosity, permeability, pore pressure, pore shape distribution, and residual brine saturation (minimum brine concentration at which flow will occur through

## Table MONPAR-1. Potentially Significant Natural Parameters

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Operational | Post-closure |
| Salado hydrology | Hydrologic properties of undisturbed Salado. Brine quantity, flux, and spatial distribution. | Properties and conditions in the far-field (undisturbed) Salado affect radionuclide containment and transport within the halite and anhydrite interbeds beyond the disturbed rock zone. | Impure halite effective porosity | Performance assessment models and calculations | 2 | 2 | N | N |
| | | | Impure halite permeability | | 2 | 2 | N | N |
| | | | Impure halite pore compressibility | | 3 | 3 | N | N |
| | | | Impure halite far-field pore pressure | | 2 | 2 | N | N |
| | | | Anhydrite permeability | | 1[c] | 1[c] | N | N |
| | | | Anhydrite pore compressibility | | 2 | 2 | N | N |
| | | | Anhydrite 2-phase flow model choice | | 2 | 2 | N | N |
| | | | Salado pore shape | | 2 | 2 | N | N |
| | | | Salado residual brine saturation | | 2 | 2 | N | N |
| | | | Salado residual gas saturation | | 2 | 2 | N | N |

## Table MONPAR-1. Potentially Signficant Natural Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Opera-tional | Post-closure |
| Salado hydrology (continued) | Hydrologic properties of undisturbed Salado. Brine quantity, flux, and spatial distribution. | Properties and conditions in the far-field (undisturbed) Salado affect radionuclide containment and transport within the halite and anhydrite interbeds beyond the disturbed rock zone. | Brine quantity (initial brine saturation)[d] | 40 CFR § 194.42(a)(5) | 3 | 3 | N | N |
| | | | Brine flux (permeabilities, porosity, pore compressibilities, model choice)[d] | | 2 | 2 | N | N |
| | | | Brine spatial distribution (initial brine saturation)[d] | | 3 | 3 | N | N |
| Salado brine | Brine composition | Brine composition affects radionuclide mobilization and repository chemistry. | Brine composition (pmH, minerals)[d] | 40 CFR § 194.42(a)(5) | 1 | 1 | N | N |
| Culebra hydrology | Hydrologic properties of undisturbed Culebra. Groundwater quantity, flux, and spatial distribution. | Properties and conditions in the undisturbed Culebra affect radionuclide transport within the Culebra in the absence of effects of human-initiated events and processes. | Transmissivity | Performance assessment models and calculations | 2 | 2 | N | N |
| | | | Advective porosity (fracture porosity) | | 2 | 2 | N | N |
| | | | Half matrix block length (fracture spacing) | | 1 | 1 | N | N |

## Table MONPAR-1. Potentially Signficant Natural Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Operational | Post-closure |
| Culebra hydrology (continued) | Hydrologic properties of undisturbed Culebra. Brine quantity, flux, and spatial distribution. | Properties and conditions in the undisturbed Culebra affect radionuclide transport within the Culebra in the absence of effects of human-initiated events and processes. | Diffusional porosity (matrix porosity) | Performance assessment models and calculations | 2 | 2 | N | N |
| | | | Longitudinal dispersivity | | 3 | 3 | N | N |
| | | | Climate change index | | 3 | 3 | N | N |
| | | | Groundwater quantity (initial brine saturation)[d] | 40 CFR § 194.42(a)(5) | 3 | 3 | N | N |
| | | | Groundwater flux (transmissivity, fracture and matrix porosity, fracture spacing and index, dispersivity, climate index)[d] | | 2 | 2 | Y | Y |
| | | | Groundwater spatial distribution (initial brine saturation)[d] | | 3 | 3 | N | N |
| Culebra groundwater | Groundwater (brine) composition | Groundwater composition may affect radionuclide transport. | Groundwater composition (pmH, minerals)[d] | 40 CFR § 194.42(a)(5) | 3 | 3 | Y | N |

## Table MONPAR-1. Potentially Signficant Natural Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Opera-tional | Post-closure |
| Castile hydrology | Hydrologic properties of undisturbed Castile. Brine quantity, flux, and spatial distribution. | Properties and conditions in the undisturbed Castile may affect direct releases from human-initiated drilling events. | Brine volume in reservoir | Performance assessment models and calculations | 1[e] | 1[e] | N | N |
| | | | Brine reservoir volume selection index | | 1[e] | 1[e] | N | N |
| | | | Brine reservoir pressure | | 1[e] | 1[e] | N | N |
| | | | Brine reservoir permeability | | 1[e] | 1[e] | N | N |
| | | | Brine reservoir rock compressibility | | 1[e] | 1[e] | N | N |
| | | | Brine quantity (brine volume)[d] | 40 CFR § 194.42(a)(5) | 1[e] | 1[e] | N | N |
| | | | Brine flux (permeability, pressure, porosity, compressibility)[d] | | 1[e] | 1[e] | N | N |
| | | | Brine spatial distribution (reservoir volume, rock volume)[d] | | 1[e] | 1[e] | N | N |

## Table MONPAR-1. Potentially Signficant Natural Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Operational | Post-closure |
| Castile brine | Brine composition | Brine composition may affect repository chemistry following human-initiated drilling events which penetrate the Castile. | Brine composition (pmH, minerals)[d] | 40 CFR § 194.42(a)(5) | 2 | 2 | N | N |
| Temperature distribution | Temperature distribution in the disposal system | Natural temperature gradients may cause physical and chemical processes and conditions that enhance radionuclide transport | Natural temperature distribution (not explicitly represented through parameters) | 40 CFR § 194.42(a)(7) | 3 | 3 | N | N |

[a] Significance legend: 1 - high, 2 - medium, 3 - low.
[b] See Appendix MON for monitoring program.
[c] Significant only in E2 intrusion. Significance is 2 in all other cases.
[d] The parameters listed in parentheses are among those used to calculate or model this property. Potentially significant parameters are also addressed separately.
[e] Significant only in E1 or E1E2 intrusions. Significance is 3 in all other cases.

the halite). Conceptually, this assumption of constant properties is based on observations of compositional and structural regularity in layers exposed by the repository and on the inference that there is little variation in large-scale averages of rock or flow properties across the disposal system. Effective porosity, permeability, pore pressure, pore shape distribution, and residual brine saturation are varied in the performance assessment models to account for observed spatial variations. Observed pore pressures are elevated above hydrostatic. In the models, they are also below lithostatic pressures; this is consistent with data collected during Waste Isolation Pilot Plant (WIPP) site experimental observations.

In summary, variable hydrologic parameters which are used to calculate **brine flux** in the intact Salado halite are **effective porosity**, **permeability**, **pore pressure**, and **pore compressibility**. Variable parameters describing the anhydrite interbeds are **effective porosity**, **permeability**, and **pore compressibility**. The **choice of model for 2-phase flow** in the anhydrite interbeds is used to accommodate the potential applicability of either of two models in predicting flow. Variable parameters common to both materials are **residual brine saturation**, **residual gas saturation**, and **pore shape distribution**. These parameters are subjected to LHS to incorporate the effects of their variability into the performance assessment calculations. These parameters are moderately significant, as they govern brine flow between the Salado and the DRZ.

**Brine quantity** within the Salado is estimated at 1 to 2 percent by volume. There is some variation in **spatial distribution**: the thin clay seams have been observed by Deal et al. (1993) to contain up to 25 to 29 percent brine by volume (Section 2.2.1.3). This brine may move toward areas of low pressure, such as the repository (see discussion of hydrologic properties of the DRZ in Section MONPAR.3.3). Flow in the intact Salado occurs only in response to pressure gradients; these do not occur in the undisturbed Salado. Much of the brine appears to be completely immobilized within the salt. Additional information is available in Appendix GCR. Brine quantity and spatial distribution are incorporated into the performance assessment models through the parameters described above.

### *MONPAR.2.2 Salado Brine Composition*

*Composition of Salado brines has been well established through investigations. Brine composition is significant and is incorporated into performance assessment calculations.*

*Based on the extensive experimental evidence collected, there is no indication that Salado brine composition will change over the regulatory period; thus it will not be routinely monitored during the operational period nor during the postclosure period.*

The composition of Salado brines has been well established through investigations over the past 15 years. Two primary brines represent the Salado: Brine A and Brine SPC (Brush, 1990). The relevant properties of both brines are incorporated into the performance assessment models through their effects on repository chemistry (MONPAR.3.7 and Appendix SOTERM). The chemical conditions in the repository, including the pmH, are assumed to be controlled by equilibrium between minerals (that is, magnesium oxide, Salado halite, and anhydrite present in interbeds), brine present, and waste. The pmH in this system with Salado brine will be about 9.4, and the carbon dioxide fugacity will be low and will be determined by the equilibrium system. The effects of magnesium oxide on repository chemistry are discussed further in MONPAR.3.7.

Given the geologic stability of the Salado and the age of the brine, overall **brine composition** is not expected to change significantly over the time scale of repository operations or, indeed, over the time scale relevant to system performance prediction.

### *MONPAR.2.3 Culebra Hydrology*

*Hydrologic properties of the undisturbed Culebra Member of the Rustler Formation exhibit spatial variability and are incorporated into performance assessment through both fixed values and parametric ranges which are consistent with experimental observations to date. Variations in some of the parameters are significant to system performance, as noted below.*

*The hydrologic properties of the undisturbed Culebra are not expected to change during the regulatory period, thus they will not be monitored during the operational period nor during the postclosure period.*

The Culebra is a fractured dolomite with nonuniform properties both horizontally and vertically. Hydrologic properties of the Culebra become important during consideration of pathways for radionuclide migration resulting from inadvertent human intrusion. While undisturbed release to the Culebra are possible, modeling shows that the most likely source for radionuclide release to the Culebra via an abandoned borehole that intersects the repository where plug materials have failed over time due to natural degradation processes. If radionuclides are introduced into the Culebra, they may be transported from the point of introduction by natural **groundwater (brine) flux** through the Culebra.

In performance assessment, the spatial distribution of **transmissivity** in the Culebra is moderately significant, as are assumptions about fracture or matrix flow and processes that may occur that retard radionuclide transport (Section MONPAR.3.10). As described in Section 6.4.6.2, the spatial variation in transmissivity observed in the Culebra (Section 2.2.1.4.1.2) is retained in performance assessment and incorporated into the calculation scheme through use of a set of transmissivity fields which honor an extensive set of experimental data. Use of a large number of transmissivity fields is a statistically sound method for characterizing the uncertainty associated with transmissivity in the Culebra.

There is considerable variability in the structure and size of porous features in the Culebra, including fractures (of a variety of dimensions and interconnectedness), vuggy zones, and inter- and intragranular porosity. The principal flow occurs within those features with the high permeability. Slower flow rates and diffusion are primary processes in the lower permeability features. The Culebra is conceptualized as having two types of porosity, advective and diffusive. Spatial variation in measured properties and uncertainties in the parameters is moderately significant and is captured through the use of LHS sampling for **advective (fracture) porosity, half matrix block length (fracture spacing), diffusive (matrix) porosity**, and **longitudinal dispersivity**. Advective porosity represents the porous features in which flow occurs. Advective porosity values are low, which is representative of flow in fractures. Diffusive porosity represents those porous features in which no flow is assumed to occur and diffusion occurs. Diffusive porosities are large relative to advective porosity, representative of the vugs, interparticle, and intercrystalline porosity of the bulk rock.

**Groundwater (brine) quantity** and **spatial distribution** are calculated quantities that are incorporated into the groundwater basin model of the units above the Salado (Section 2.2.1.4). Climate change effects have been incorporated into the flow model through use of a **climate change index** simulating increased recharge at the water table resulting from a cooler, wetter climate. The increased recharge is modeled through the groundwater velocity field in the Culebra. Variation in the climate change index is captured through the use of LHS sampling in performance assessment and is not significant to system performance.

### *MONPAR.2.4 Culebra Groundwater Composition*

*Culebra groundwater is less saline than Salado and Castile brines. The Culebra groundwater is spatially variable, and its composition has been well established through investigations. Groundwater composition is incorporated into performance assessment calculations; however it is not significant to performance.*

*Based on extensive experimental evidence there is no indication that Culebra groundwater composition will change over the regulatory period; however, monitoring would provide information that is relevant to a comprehensive environmental monitoring program.*

There is considerable variation in groundwater chemistry in the Culebra. Four zones, each with its characteristics, have been identified (Section 2.4.2.1). The groundwater in each of these zones has been well characterized. Note that the fluid in the Culebra is referred to as groundwater to differentiate it from the more saline brines found in the Salado and Castile.

Given the observed geologic stability of the Culebra and the age of the groundwater, overall **brine (groundwater) composition** is not expected to change significantly over the time scale of repository operations or, indeed, over the time scale important to disposal system performance.

### *MONPAR.2.5 Castile Hydrology*

*The Castile Formation underlying the WIPP may contain reservoirs of pressurized brine. This is incorporated into performance assessment through use of input parameters that address hydrologic properties and the probability that a reservoir will be encountered during* *an intrusion event. The hydrologic properties are significant to disposal system performance in such an intrusion event. The Castile is not significant to system performance except for the brine reservoirs.*

*There is no indication that the properties of the undisturbed reservoirs will change over the regulatory period although the assumpiton is made in the modeling that intrusions into brine reservoirs leads to their eventual depletion. It is not possible to completely define the location and extent of brine reservoirs without jeopardizing the integrity of the disposal system.*

The Castile underlying the WIPP is dominated by low-permeability anhydrite and halite zones, with isolated regions of higher permeability that may contain pressurized brine. Hydraulic tests indicate these brine reservoirs are limited in extent, but their location and dimensions are uncertain, as described in Section 6.4.12.6. The probability of encountering a reservoir in any intrusion event is discussed in MONPAR.4.1. The presence of the brine and the parameters describing reservoir properties are significant to repository performance only in the event of inadvertent human intrusion into the repository and underlying brine reservoir (the E1 intrusion event described in Section 6.3.2.2.1).

The properties of the brine reservoir used in performance assessment include the **pressure**, **permeability**, **rock compressibility**, and **brine volume** (quantity). As described in Section 6.4.8, five possible reservoir **brine volumes** are used in calculating the consequences of first penetration of a reservoir by an exploratory borehole. An **index** is used to randomly select the volume of the reservoir that may be encountered during an intrusion event. In the performance assessment calculations, the porosity of the brine reservoir is set such that the reservoir brine volume is contained in the constant rock volume used in the model (that is, the **spatial distribution** of the brine). A brine reservoir is assumed to exist beneath the waste panels, and it is assigned properties that include some sampled parameters.

### *MONPAR.2.6 Castile Brine Composition*

*Composition of brines from two Castile brine reservoirs is moderately significant and is incorporated into performance assessment calculations.*

*There is no evidence to suggest that the brine composition will change over the regulatory period. It is not possible to further investigate composition of any brine which may be present below the repository without jeopardizing the integrity of the disposal system. Therefore no further investigations or monitoring will be performed during the operational period nor during the postclosure period.*

Two brines encountered in the Castile (WIPP-12 and ERDA-6) differ from each other, but both are nearly saturated with respect to halite (Brush, 1990). The relevant aspects of the ERDA-6 **brine composition** are incorporated into the performance assessment models through its effect on repository chemistry (MONPAR.3.7 and Appendix SOTERM). Under conditions where pressurized Castile brine enters the repository, the chemical conditions in the repository, including the pmH, are assumed to be controlled by equilibrium between minerals (that is, magnesium oxide, halite, and anhydrite present in interbeds), brine present, and waste. The pmH in the system with Castile brine will be approximately 9.9. The carbon dioxide fugacity will accordingly be maintained at low levels and will be determined by the equilibrium system. This will serve to limit radionuclide solubilities. The effects of magnesium oxide on repository chemistry are discussed further in MONPAR.3.7.

### *MONPAR.2.7 Natural Temperature Distribution*

*Natural geological thermal gradients have been characterized and are not significant: they will not affect repository performance, either directly by affecting the containers and repository chemistry, or indirectly by altering fluid flow through the Salado or the Culebra. Therefore natural thermal gradients will not be monitored during the operational period nor during the postclosure period.*

As described in Appendix SCR (Section SCR.1.2.2.3), the geothermal gradient in the region of the WIPP has been measured at about 50°C per mile (30°C per kilometer). Given the generally low permeability in the region, and the limited thickness of units in which groundwater flow occurs (for example, the Culebra), natural convection will not have a significant effect on groundwater flow. No natural FEPs have been identified that could significantly alter the **temperature distribution** of the disposal system or give rise to thermal effects on groundwater flow.

## MONPAR.3 Potentially Significant Parameters that Describe Waste- and Repository-Induced Properties and Processes

The parameters that describe waste- and repository-induced properties and processes that were considered in the analysis fall into ten groups:

- Stresses and extent of deformation of the surrounding roof, walls, and floor of the waste disposal room; mechanical properties and behavior of the halite during creep closure.

- Initiation or displacement of major brittle deformation features in the roof or rock; mechanical properties and behavior of brittle rock (anhydrites) during creep closure.

- Altered hydrologic properties of the Salado in the DRZ surrounding the repository, including properties which govern brine quantity, flux, and spatial distribution.

- Mechanical and hydrologic properties of the disposal room (and the waste in it) in response to repository conditions (mechanical properties of backfill are considered separately).

- Properties of backfilled material, including porosity, permeability, and degree of compaction and reconsolidation.

- Gas generation processes and rates; quantity and composition of gas in the disposal room.

- Disposal room chemistry and radionuclide source term; chemical composition of the brine, and interactions between the waste, brine, gas, and backfill.

- Temperature distribution in the repository.

- Shaft seal system performance.

- Mechanisms for radionuclide transport and retardation outside the repository.

The results of the DOE's analysis are presented in Table MONPAR-2. The parameters describing the waste- and repository-induced properties and processes are discussed in the following section.

### *MONPAR.3.1 Creep Closure*

*Creep closure of the repository will occur, and is included within compliance assessment and performance assessment models as a control on waste consolidation and other time-dependent disposal room conditions. The individual creep closure related parameters are not significant to performance assessment. Sufficient data have been collected for the purposes of verifying the underlying rock mechanics models as discussed subsequently. The numerical models of the repository used in performance assessment are based upon assumptions about long-term behavior that are not applicable to behavior during the operational period.*

*Further monitoring of creep closure and stress would not provide information that is useful for calculating disposal system performance, nor would it lead to additional confidence in the performance assessment models. However, monitoring creep closure would provide information that is relevant to repository operations (Section 7.2.3.1).*

Since the start of excavation at the WIPP, salt creep has led to deformation of the roof, walls and floor of the openings. Extensive monitoring of the resulting creep closure and **extent of deformation** has taken place over more than a decade, through measurements within the excavated rooms, and additional monitoring has been conducted in boreholes drilled from the repository. Data acquired from these measurements have been used to calculate **stresses** and to derive, calibrate and verify conceptual and numerical models of salt creep around excavations (for example, see Munson et al. 1989a,b; Munson and DeVries 1991). The models incorporate individual parameters such as **shear modulus**, **Young's modulus** and **Poisson's ratio**, and thermal properties such as **specific heat** to calculate extent of creep and dislocation.

## Table MONPAR-2. Potentially Signficant Waste- and Repository-Induced Parameters

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Opera-tional | Post-closure |
| Creep closure | Mechanical properties and behavior of the halite during creep closure. Stresses and extent of deformation of the surrounding roof, walls, and floor of the waste disposal room. | In response to the pressure gradient caused by the excavation and potential repository pressurization, the salt surrounding the repository will deform and creep. Fractures will also form in the salt, creating a disturbed rock zone (DRZ) around the repository (hydrologic properties of the DRZ are discussed separately). | Stresses (shear modulus, Young's modulus, Poisson's ratio, specific heat)[c] | 40 CFR § 194.42(a)(2) | 3 | 3 | Y | N |
| | | | Extent of deformation (shear modulus, Young's modulus, Poisson's ratio, specific heat)[c] | | 3 | 3 | Y | N |
| Major deformation features in surrounding rock | Mechanical properties and behavior of brittle rock during creep closure. Initiation or displacement of major brittle deformation features in the roof or surrounding rock. | In response to the pressure gradient caused by the excavation and potential repository pressurization, the brittle anhydrite interbeds are likely to fracture. Such fractures could potentially extend beyond the DRZ, forming large-scale fractures and causing subsidence. | Initiation of brittle deformation features (fracture initiation pressure, increment for full fracturing)[c] | 40 CFR § 194.42(a)(3) | 3 | 3 | Y | N |
| | | | Displacement of major brittle deformation features (not explicitly represented through parameters) | | 3 | 3 | Y | N |

## Table MONPAR-2. Potentially Signficant Waste- and Repository-Induced Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Operational | Post-closure |
| Salado hydrology near the repository (DRZ) | Hydrologic properties of disturbed Salado in the DRZ near the repository. Brine quantity, flux, and spatial distribution. | Altered hydrologic properties in the DRZ (halite and anhydrite) may enhance fluid transport into and out of the waste disposal area. | DRZ permeability | Performance assessment models and calculations | 2 | 2 | N | N |
| | | | DRZ effective porosity | | 2 | 2 | N | N |
| | | | Brine flux (DRZ effective porosity and permeability, fracture permeability enhancement)[c] | 40 CFR § 194.42(a)(5) | 2 | 2 | N | N |
| | | | Brine quantity and spatial distribution (DRZ initial brine saturation)[c] | | 3 | 3 | N | N |
| Disposal room properties | Mechanical and hydrologic properties of the disposal room (and the waste in it) in response to repository conditions | Disposal room properties affect fluid flow in and out of the repository, and radionuclide migration out of the repository. | Waste area residual gas saturation | Performance assessment models and calculations | 2[d] | 2[d] | N | N |
| | | | Waste area residual brine saturation | | 2[d] | 2[d] | N | N |
| | | | Brine wicking | | 2 | 2 | N | N |
| | | | Waste area permeability | | 2 | 2 | N | N |

## Table MONPAR-2. Potentially Signficant Waste- and Repository-Induced Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Opera-tional | Post-closure |
| Backfill mechanical properties | Properties of backfilled material, including porosity, permeability, and degree of compaction and reconsolidation | Backfill present in the disposal room may provide sufficient mechanical strength to retard creep closure of the surrounding halite. Backfill may also alter fluid flow in the disposal room. | Backfill porosity | 40 CFR § 194.42(a)(1) | 3 | 3 | N | N |
| | | | Backfill permeability | | 3 | 3 | N | N |
| | | | Degree of backfill compaction | | 3 | 3 | N | N |
| | | | Backfill reconsolidation | | 3 | 3 | N | N |
| Gas generation | Gas generation processes and rates. Quantity and composition of gas in the disposal room. | Gas pressure may retard disposal room closure and enhance fluid flow and radionuclide migration out of the disposal room. Gas composition affects brine composition and disposal room chemistry. | Rate of steel corrosion under inundated conditions with carbon dioxide present | Performance assessment models and calculations | 3 | 3 | N | N |
| | | | Rate of steel corrosion under inundated conditions without carbon dioxide | | 2 | 2 | N | N |
| | | | Rate of microbial degradation under inundated conditions | | 3 | 3 | N | N |
| | | | Rate of microbial degradation under humid conditions | | 3 | 3 | N | N |

## Table MONPAR-2. Potentially Signficant Waste- and Repository-Induced Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Opera-tional | Post-closure |
| Gas generation (continued) | Gas generation processes and rates. Quantity and composition of gas in the disposal room. | Gas pressure may retard disposal room closure and enhance fluid flow and radionuclide migration out of the disposal room. Gas composition affects brine composition and disposal room chemistry. | β-factor for microbial degradation process | Performance assessment models and calculations | 3 | 3 | N | N |
| | | | Probability factor for different types of microbial degradation | | 3 | 3 | N | N |
| | | | Gas quantity (rates of corrosion and microbial degradation, probability of microbial degradation)[c] | 40 CFR § 194.42(a)(6) | 2 | 2 | Y | N |
| | | | Gas composition (hydrogen, carbon dioxide)[c] | | 3 | 3 | Y | N |
| Disposal room chemistry | Chemical composition of brine in disposal room.<br>Chemical interactions between waste, brine, gas, and backfill.<br>Actinide source term. | Brine composition and properties affect actinide solubility and colloid formation and stability. Gas composition affects brine composition. Backfill controls composition of gas and brine. | Choice of radionuclide oxidation state distribution | Performance assessment models and calculations | 1 | 1 | N | N |

## Table MONPAR-2. Potentially Signficant Waste- and Repository-Induced Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Opera-tional | Post-closure |
| Disposal room chemistry (continued) | Chemical composition of brine in disposal room.<br>Chemical interactions between waste, brine, gas, and backfill.<br>Actinide source term. | Brine composition and properties affect actinide solubility and colloid formation and stability. Gas composition affects brine composition. Backfill controls composition of gas and brine. | Solubility of Am(III), Cm(III), Pu(III), Pu(IV), Th(IV), U(IV), Np(IV), Np(V), and U(VI) in Salado brine[e] | Performance assessment models and calculations | 1 | 1 | N | N |
| | | | Solubility of Am(III), Cm(III), Pu(III), Pu(IV), Th(IV), U(IV), Np(IV), Np(V), and U(VI) in Castile brine[e] | | 1 | 1 | N | N |
| | | | Concentration of humic colloids containing III, IV, V, and VI actinides (expressed as a fraction of concentration of dissolved III, IV, V, and VI actinides, respectively) in Salado brine | | 1 | 1 | N | N |

## Table MONPAR-2. Potentially Signficant Waste- and Repository-Induced Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment [a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Opera-tional | Post-closure |
| Disposal room chemistry (continued) | Chemical composition of brine in disposal room.<br>Chemical interactions between waste, brine, gas, and backfill.<br>Actinide source term. | Brine composition and properties affect actinide solubility and colloid formation and stability. Gas composition affects brine composition. Backfill controls composition of gas and brine. | Concentration of humic colloids containing III, IV, V, and VI actinides (expressed as a fraction of concentration of dissolved III, IV, V, and VI actinides, respectively) in Castile brine | Performance assessment models and calculations | 1 | 1 | N | N |
| Shaft seal system | Performance of shaft seal system. | Shaft seals help provide long-term waste containment in the repository. | Clay member permeability | Performance assessment models and calculations | 2 | 2 | N | N |
| | | | Concrete member permeability | | 2 | 2 | N | N |
| | | | Asphalt member permeability | | 2 | 2 | N | N |
| | | | Shaft DRZ permeability | | 2 | 2 | N | N |
| | | | Index for selecting crushed salt seal component permeability to represent consolidation | | 1 | 1 | N | N |

## Table MONPAR-2. Potentially Signficant Waste- and Repository-Induced Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Opera-tional | Post-closure |
| Shaft seal system (continued) | Performance of shaft seal system. | Shaft seals help provide long-term waste containment in the repository. | Seal residual gas saturation | Performance assessment models and calculations | 3 | 3 | N | N |
| | | | Seal residual brine saturation | | 3 | 3 | N | N |
| | | | Seal pore shape | | 3 | 3 | N | N |
| Temperature distribution | Temperature distribution in the repository | Waste- and repository-induced temperature gradients may cause physical and chemical processes and conditions that enhance radionuclide transport | Waste- and repository-induced temperature distribution (not explicitly represented through parameters) | 40 CFR § 194.42(a)(7) | 3 | 3 | N | N |
| Radionuclide transport | Mechanisms for transport and retardation outside the repository. | Transport is governed by the form of the radionuclide and the physical and chemical features of the formation. | Distribution coefficients for dissolved radionuclides in the Salado | Performance assessment models and calculations | 3 | 3 | N | N |
| | | | Distribution coefficients for colloidal radionuclides in the Salado | | 3 | 3 | N | N |

## Table MONPAR-2. Potentially Signficant Waste- and Repository-Induced Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment [a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Operational | Post-closure |
| Radionuclide transport (continued) | Mechanisms for transport and retardation outside the repository. | Transport is governed by the form of the radionuclide and the physical and chemical features of the formation. | Distribution coefficients for dissolved Am(III), Pu(III), Pu(IV), Th(IV), U(IV), and U(VI) in the Culebra | Performance assessment models and calculations | 1 | 1 | N | N |

[a] Significance legend: 1 - high, 2 - medium, 3 - low.

[b] See Appendix MON for monitoring program.

[c] The parameters listed in parentheses are among those used to calculate or model this property. Potentially significant parameters are also addressed separately.

[d] Significant only in E1 intrusions: E1, E2, and E1E2. Significance is 3 in all other cases.

[e] Solubility distributions are calculated for each actinide using the FMT model and code.

The detailed rock mechanics models of salt creep have been used to derive simplified models for the DRZ and repository for use in performance assessment calculations (Section 6.4.3.1, Appendix PORSURF). Although based on rock mechanics, these models of repository behavior are also based on a number of assumptions about long-term behavior that will not be applicable to modeling behavior during the preclosure period (for example, the models assume that the waste containers have little strength and do not impede closure of the disposal room).

### *MONPAR.3.2 Major Deformation Features*

*The initiation or displacement of major brittle deformation features in the roof or surrounding rock, beyond that already accounted for in performance assessment calculations, is not significant to the containment of waste. The individual parameters that are used in modeling the mechanical behavior of brittle anhydrite interbeds are not significant to performance assessment; the parameters that are used in modeling hydrological effects are discussed in MONPAR.3.3.*

*Monitoring mechanical behavior of the interbeds would not provide information that is useful for calculating system performance, nor would it lead to additional confidence in the performance assessment models. However, monitoring would provide information that is relevant to repository operations (Section 7.2.3.1).*

Because the Salado is not composed of pure halite, and because the rate of deformation near the repository may be too great to be accommodated entirely by salt creep, other deformation mechanisms will accompany salt creep. These other mechanisms can be collectively classified as brittle deformation. Should these mechanisms occur, they will result in the extension of the DRZ around the repository. This potentially increases the instability of the DRZ could to lead to localized roof falls in the first few hundred years (Appendix SCR, Section SCR.2.3.3). In such cases, development of the DRZ may be sufficient to disrupt the anhydrite layers above the repository, which may create a zone of rock containing anhydrite extending from the interbeds toward a waste-filled room. **Brittle deformation features** (fractures) may be induced as the rock stress and strain distributions evolve because of creep, or in response to fluid pressure in the repository. Because of uncertainty in the process by which the disposal room DRZ heals, the flow model used in the performance assessment assumes that a higher-permeability zone remains for the long term. Thus, the potential effects of roof falls on flow paths are accounted for in performance assessment calculations through the parameters describing the hydrologic properties of the DRZ (MONPAR.3.3). In the long term, the effects of roof falls in the repository will not be significant because salt creep will reduce the void space and the potential for roof falls; the salt creep will also consolidate roof material that has fallen into the rooms.

Subsidence through salt creep or roof collapse associated with excavation or repository closure might affect the hydrologic properties of units above the repository and might cause large-scale rock fracturing (**displacement of major brittle deformation features**) between the repository horizon and the surface (Appendix SCR, Section SCR.2.3.4). The amount of subsidence that can occur as a result of salt creep closure in the waste-filled and sealed areas of the repository depends on the volume of extracted rock, the initial and compressed porosities of various emplaced materials, the amount of inward creep of the repository walls, and the gas and fluid pressures within the repository. The DOE (Westinghouse 1994) has analyzed potential excavation-induced subsidence at the WIPP. For an empty repository, the DOE estimated the maximum potential subsidence at the surface to be less than 2 feet (0.62 meter). Maximum subsidence at the depth of the Culebra was estimated to be less than 1.8 feet (0.56 meter), and the maximum horizontal displacement at the depth of the Culebra was estimated to be less than 0.08 feet (0.2 meter), with a maximum horizontal strain of 0.007 percent. The induced strains will be uniformly distributed because no known faults or discontinuities occur in the vicinity of the WIPP. Strains of this magnitude would not be expected to cause cracking or extensive fracturing.

The DOE (Westinghouse 1994) also reported investigations of subsidence associated with potash mining operations located near the WIPP site to gain insight into the expected subsidence conditions at the WIPP. Subsidence over potash mines in the area will be much greater than at the WIPP because of the significant differences in stratigraphic position, depth, extraction ratio, and layout. The proposed WIPP rock extraction ratio is about 22 percent, as compared to over 65 percent for the lowest extraction ratios within local potash mines investigated by DOE. Also, the WIPP site is located stratigraphically much lower than the lowest potash mine, which is near the base of the McNutt Potash Zone (hereafter referred to as the McNutt). The base of the McNutt is about 490 feet (150 meters) above the repository horizon.

The reported maximum total subsidence at potash mines is about 5 feet (1.5 meters). This level of subsidence has been observed to have caused surface fractures. However, the DOE found no evidence that subsidence over potash mines had caused fracturing sufficient to connect the mining horizon to water-bearing units or the surface. The level of disturbance caused by subsidence above the WIPP repository will be less than that associated with potash mining and thus, by analogy, will not create fluid flow paths between the repository and the overlying units.

As a result of numerical analyses and observations of subsidence associated with potash mines, fracturing within units overlying the Salado and surface displacements caused by subsidence associated with repository closure are considered insignificant. The potential for subsidence to create fluid flow paths between the repository and units overlying the Salado is also considered insignificant, as it has low probability of occurrence over 10,000 years.

### *MONPAR.3.3 Hydrologic Properties in the DRZ*

*The presence of a DRZ surrounding the repository has been incorporated into performance assessment calculations. The properties of the DRZ have been well characterized; they include altered hydrologic properties which are expected to enhance near-field fluid flow both to and from the repository. The initial conditions and enhanced fluid flow are moderately significant to disposal system performance. In an effort to simplify the calculations, the effects* *are...properties of the DRZ. This is believed to be a conservative choice with respect to the ultimate impact on predicted release.*

*Monitoring the DRZ hydrologic properties would not provide relevant information or verify assumptions used in performance assessment; therefore they will not be monitored during the operational period nor during the postclosure period.*

Construction of the repository has caused a local change in stress field and has altered the permeability and effective porosity of the nearby rock around the repository. The increases in permeability and porosity in the interbeds are not expected to be completely reversible with creep closure of the disposal rooms. In addition, increased fluid pressure in the repository is expected to cause dilation and fracturing of the anhydrite interbeds. If they occur in performance assessments, these changes will further increase the permeability and porosity of the interbeds, providing enhanced pathways for flow of gas and brine (**brine flux**) between the waste-filled rooms and the nearby interbeds. The model of the DRZ used in performance assessment (described in Section 6.4.5.3) includes permanently increased **permeability** (to enhance fluid flow), and an increased effective **porosity** (reflecting observed changes in the DRZ and long-term conditions consistent with increased permeability). The performance assessment treatment of the DRZ creates a permanent high-permeability region that does not significantly impede flow between the repository and affected interbeds.

In the computational models, **brine quantity** and **spatial distribution** are calculated using the **initial brine saturation** and other parameters describing initial conditions for the simulation of the regulatory period. These parameters describe properties that are consistent with modeling assumptions and with observed conditions in that the DRZ is assumed to be initially fully brine-saturated near the repository. Excavation and waste emplacement operations result in partial drainage of the DRZ, subsequent evaporation of drained brine into mine air, followed by removal from the modeled system by air exchanged to the surface. The duration of the modeled operations is five years, simulating the shortest expected time between excavation and sealing of an individual panel. Thus the modeled DRZ has the highest reasonable initial brine saturation.

### *MONPAR.3.4 Hydrologic Properties in the Disposal Room*

*Mechanical and hydrologic properties of the disposal room are incorporated into performance assessment as they affect gas generation and fluid flow into and out of the repository. These properties and parameters are moderately significant to disposal system performance. Additional properties are significant in the event of intrusion into the repository; these are discussed in MONPAR.4.2. The conceptual model of disposal room behavior is based on extensive experimental data which support a number of assumptions about long-term behavior that will not be applicable during the preclosure period.*

*The closed disposal room will not achieve the expected long-term properties predicted in performance assessment during the operational or active control periods. Therefore,* *monitoring the mechanical and hydrologic properties would not provide relevant information or verify assumptions used in performance assessment. Thus the disposal room properties will not be monitored during the operational period nor during the postclosure period.*

Creep closure of waste disposal areas will cause their volume to decrease as the Salado deforms to consolidate and encapsulate the waste. This results in an associated change to the waste porosity. Resistance to creep closure is a function of both waste strength and fluid pressure. The amount of waste consolidation that occurs and the time it takes are governed by properties of the waste (waste strength, modulus, etc.), properties of the surrounding rock, the dimensions and location of the room, and the quantities of fluids present in the room. As described in Section 6.4.3.1, the closure process is modeled in terms of a porosity surface relating waste porosity to gas quantity, fluid pressure, and time under various conditions which affect gas generation.

In order to simulate long-term behavior, all waste containers are assumed to be breached at the time of final facility closure, allowing the contents to be immediately available for reactions which could generate gas. The effects of **wicking** are incorporated to account for the possibility of increased brine contact with the waste. The **permeability** of the waste is maintained in the model at a value representative of the average value of the compacted waste. Maximizing brine contact with the waste also increases radionuclide solubility and is consistent with assumptions in the conceptual models of repository chemistry (Section 6.4.3.4 and MONPAR.3.7). The **residual brine saturation** and **residual gas saturation** indicate the brine and gas saturation (respectively) at which brine or gas will flow through the waste; below these saturations the brine and gas are immobile. The variations in these parameters reflect the variety of wastes present in the repository.

These waste properties are moderately significant in the event of inadvertent human intrusion into the repository, as they will have some effect on the direct and long-term releases by affecting fluid flow through the repository. Direct and long-term releases resulting from inadvertent human intrusion are discussed in Sections MONPAR.4.2 and MONPAR.4.3, respectively.

### *MONPAR.3.5 Backfill Properties*

*The mechanical and hydrologic properties of the backfill are not significant to the performance assessment. Therefore, they will not be monitored during the operational or postclosure periods. Chemical control and chemical properties of the backfill are addressed in Section MONPAR.3.7.*

The principal function of the backfill to be emplaced in the WIPP will be to control the chemical conditions in the disposal rooms resulting in a reduced potential for radionuclides to dissolve in brine. The backfill material will also have beneficial mechanical and hydrologic effects.

The amount of subsidence that can occur as a result of salt creep closure depends on the extraction ratio, the initial and compressed porosities of emplaced materials, the amount of inward creep of the repository walls, and the gas and fluid pressures within the repository. The DOE (Westinghouse 1994) has analyzed potential excavation-induced subsidence and the mechanical benefits of backfilling at the WIPP. Results of the DOE's study show that backfill emplacement would not significantly decrease subsidence in the waste emplacement area.

Similarly, because the backfill volume will be less than the waste volume, the reduction in average room permeability and effective porosity provided by the backfill will be insignificant. After waste emplacement, room permeability and effective porosity will be controlled essentially by the waste properties, the amount of salt creep, and the gas and fluid pressures. Thus, the backfill **porosity**, **permeability**, **degree of compaction**, and **reconsolidation** will have an insignificant effect on hydrologic conditions in the disposal rooms. Further, any deviations from expected performance will be beneficial to disposal system performance.

### *MONPAR.3.6 Gas Generation*

*Gas generated in the repository may retard creep closure, may fracture the anhydrite interbeds in the DRZ (enhancing fluid flow), and may enhance direct releases (MONPAR.4.2) These effects are moderately significant and are accounted for in performance assessment. Gas composition (carbon dioxide concentration) and the corrosion rate of metals are controlled chemically by the backfill and are not significant. Gas generation is moderately significant to system performance. The conceptual model of gas generation processes is based on experimental data and incorporates a number of assumptions about long-term behavior that will not be applicable during the operational period (such as anoxic conditions).*

*Monitoring the quantity and composition of gas generated in the closed panels would not provide information that is useful for calculating system performance, nor would it lead to additional confidence in the performance assessment models.*

The major gas generation and consumption processes are incorporated into the models of the repository (Section 6.4.3.3). Gas will be produced in the repository because of a variety of chemical reactions, primarily those occurring between brine, metals, microbes, cellulosics and similar materials, plastics, and rubber materials, and by liberation of dissolved gases to the gas phase. The dominant processes are anoxic corrosion of metals in the waste containers and the waste and microbial degradation of cellulosics, plastics, and rubbers in the waste. Anoxic corrosion reactions will occur (in the presence of liquid brine) between brine and steel, aluminum, and aluminum alloys, producing hydrogen. All possible corrosion reactions are dependent on the presence of brine and decrease under alkaline conditions. The **corrosion rate** is affected by the presence of carbon dioxide produced by microbial degradation. Carbon dioxide will be controlled through reaction with the magnesium oxide (MgO) backfill (Appendix SOTERM Section SOTERM.2.2.2). Therefore, the gas in the repository will be composed primarily of hydrogen and the corrosion of steel in the absence of carbon dioxide is the primary mechanism for gas generation in the closed repository; it is moderately significant to system performance.

Microbial degradation of cellulosics may or may not occur in the repository; this uncertainty is represented in the model by a **probability factor**. The **microbial degradation rate** differs for brine-inundated and humid conditions. The **$\beta$ factor** is used to characterize the extent to which microbial-generated gases react with steel and steel corrosion products. Microbial degradation may produce a variety of gases; however, for the waste inventory and expected conditions, carbon dioxide and methane are expected to be the dominant gases generated. Radiolysis has been demonstrated by laboratory experiment and model calculations to be insignificant (Appendix SCR Section SCR.2.5.1.3.1).

The current conceptual models assign the density and viscosity of hydrogen to all generated gases. Since hydrogen is the most mobile of all the possible gas components, this assumption is both reasonable and conservative. Therefore, this assumption renders the **composition of the gas** as insignificant.

**Gas quantity** is a calculated quantity. It will affect repository pressure, which is a moderately significant parameter in other submodels of the disposal system, such as those calculating creep closure (Section 6.4.3.1), interbed fracturing (Section 6.4.5.2), two-phase flow (Section 6.4.3.2), and the radionuclide release associated with spallings during an inadvertent drilling intrusion (Section 6.4.7.1). Thus, gas quantity must be estimated and is significant to performance assessment. The model incorporates several assumptions designed to maximize gas generation in the years immediately following closure (for example, minimizing brine drainage from the DRZ by limiting the modeled operating period to five years and immediately breaching all containers). Thus, monitoring gas pressure or composition would not verify the assumptions made in the models.

### *MONPAR.3.7 Repository Chemical Conditions*

*Chemical conditions in the repository will affect radionuclide solubility; the solubility of dissolved radionuclides and stability of colloidal species are significant to system performance. The chemical conditions are controlled by interactions between the waste, abundant minerals in the brine, the backfill, and gas generated by microbial degradation in the repository. The conceptual model incorporates assumptions about long-term performance (for example, chemical constant conditions, thermodynamic equilibrium, and mixing the waste and brine) that are not applicable during the operational period.*

*The closed repository will not achieve the long-term chemical conditions (brine composition, dissolved actinide concentrations, or colloidal actinide concentrations) used in performance assessment during the operational or active control periods. Therefore, monitoring the chemical conditions will not provide relevant information or verify assumptions used in performance assessment. Chemical conditions in the repository cannot be monitored after* *decommissioning without jeopardizing repository integrity. Thus these parameters will not be monitored during the operational period nor during the postclosure periods.*

Brine composition in the repository can vary depending on the sequence of future human events. Brine from the Salado or brine from the Castile may be present in the repository in certain scenarios (Section 6.4.3.4). The compositions of these brines are discussed in MONPAR.2.2 and MONPAR.2.6, respectively. The chemical environment in the repository after closure is expected to favor lower oxidation states (that is, to be reducing). Based on experimental data (Appendix SOTERM Section SOTERM.3.4), the DOE has determined that alkaline conditions in the repository favor lower solubilities of the radionuclides (actinides).

Magnesium oxide will be added to the repository with the waste to ensure that alkaline conditions exist in the repository. The DOE will emplace enough magnesium oxide with sufficient surface area to ensure carbon dioxide uptake will exceed the carbon dioxide production rate. Therefore, it has been assumed that MgO emplaced with the waste will react with the carbon dioxide that forms, creating magnesium carbonate materials. Consequently, the fugacity of the carbon dioxide will be low. Because the processes that might cause time-dependent changes in important chemical conditions in the repository have been eliminated by addition of magnesium oxide and by the assumptions made regarding brine composition, performance assessment uses constant chemical conditions. The chemical conditions in the repository, including the pmH, are assumed to be controlled by equilibrium between minerals (that is, magnesium oxide, Salado halite, and anhydrite present in interbeds), brine present, and waste. In Salado brine, the pmH in this system will be about 9.4. In Castile brine, the pmH in this system will be about 9.9. (Appendix SOTERM Section SOTERM 2.2.2).

Radionuclides in the waste may be mobilized either by dissolution in brine, by bioaccumulation or sorption onto colloidal particles, or by condensation into colloidal forms as actinide-intrinsic colloids that could be carried by brine (Section 6.4.3.6). The dissolved actinide source term model calculates the dissolved concentration of each actinide in solution by applying the modeled solubility for the particular oxidation state, as determined by the oxidation state distribution for that actinide, at the repository conditions presented in Section 6.4.3.4. There are two possible oxidation state distributions for the actinides; each with a 50 percent chance of occurring. In the first distribution, the actinides exist in the more reduced oxidation states (reflecting extreme reducing conditions): U(IV), Np(IV), and Pu(III). In the second distribution, the radionuclides are present at higher oxidation states (reflecting less extreme reducing conditions): U(VI), Np(V), and Pu(IV). Both distributions also include Th(IV), Am(III), and Cm(III). The **oxidation state index** is used to randomly select which distribution is used in a given realization (Appendix SOTERM Section SOTERM.4). The **solubility** of the actinides in each oxidation state is calculated as a function of equilibrium between anhydrite, magnesium oxide, and brine. Thus the solubility is modeled in both **Salado and Castile brines**.

Colloidal particles may be formed in the repository through a variety of processes. The expected processes include waste degradation, microbial activity, rock decomposition, and chemical condensation. These particles may also be carried into the repository by liquids moving from the Salado or through boreholes. Because of the presence of soils, nutrients, and cellulosic substrates for microbial action in WIPP waste (Appendix BIR), humic substances and microbes will be present in disposal room brines, and may form in situ. Actinide-intrinsic colloids may form in the disposal rooms from condensation of dissolved actinides. Mineral fragments, as well as humic substances and microbes, may provide surfaces on which dissolved actinides could sorb.

Actinides associated with microbes and humics are related to the concentration of dissolved actinides in the repository through proportionality constants (that is, the **proportion of actinides in the dissolved and colloidal phases**) determined from interpretation of WIPP-relevant experiments and the literature. The relationship is not based rigorously on thermodynamic equilibrium, but is simply a relationship. The concentration of actinides associated with the Pu(IV)-polymer is a constant value determined from experimental results at the pH conditions dictated by the presence of MgO backfill. Likewise, the concentration of actinides associated with mineral colloids is also a constant value, not linked to the concentration of dissolved actinides. Actinides associated with humics and microbes represent most of the colloidal actinide source term. Consequently, the colloidal actinide source term is closely related to the dissolved actinide source term. As discussed in a later section, however, the source terms are considered separately for transport in the Culebra.

The concentrations of colloidal actinides indicated in this section are assumed to be concentrations of actinides mobilized on colloidal particles. The indicated concentrations will be entrained in moving brine. For conservatism, it is assumed that no actinides sorb onto colloidal particles that are not mobile in the repository. Thus all actinides in the repository will be present in the solid phase, dissolved in the aqueous phase, or as colloidal actinides suspended in the aqueous phase.

### *MONPAR.3.8 Temperature Distribution*

*Waste-induced and repository-induced thermal gradients in the repository are not significant: they will not affect repository performance, either directly by affecting the containers and repository chemistry, or indirectly by altering fluid flow through the Salado or the Culebra. Therefore waste- and repository-induced thermal gradients will not be monitored during the operational period nor during the postclosure period.*

Temperature in the repository may be influenced by radioactive decay, and exothermic reactions. As described in Appendix SCR (Section SCR.2.2.2), the maximum temperature increase due to radioactive decay will be in the vicinity of remote-handled transuranic waste containers; the increase is approximately 3°C. The expected repository temperature increase due to radioactive decay is less than 2°C.

The exothermic reactions anticipated in the repository are hydration of concrete material in the seals and panel closures, hydration of the magnesium oxide backfill, and temperature increases associated with hydration of the concrete in the seals and panel closures localized in and around the seals and panel closures. The seals contain a large quantity of concrete but are not located adjacent to the waste disposal panels. Salt dissipates heat quickly; thus the effects are also expected to be minimal. Temperature increases due to hydration of backfill are expected to be insignificant and will be further limited by low brine inflow rates. The maximum temperature increase in the repository due to magnesium oxide hydration reactions will be approximately 5°C (Attachment MONPAR-1). The total temperature rise (due to radioactive decay and exothermic reactions) is estimated to be less than 7°C.

### *MONPAR.3.9 Shaft Seal System*

*Shaft seals assure waste containment in the repository. They are incorporated into performance assessment and their hydrologic properties are moderately significant to disposal system performance.*

*The seals will not be emplaced until the repository is decommissioned; thus their performance cannot be monitored during the operational period. The performance of the seals cannot be monitored after emplacement without jeopardizing the integrity of the disposal system. Thus the seal performance will not be monitored during the operational period or during the postclosure period.*

The seal system consists of multiple components emplaced in the shaft: **clay**, **concrete**, **asphalt**, and crushed salt. A **DRZ** has formed around each shaft in response to the deviatoric stress created by excavation of the shafts; this DRZ has enhanced hydrologic properties similar to those in the DRZ surrounding the disposal rooms. The effective permeability of each seal component is a function of the **permeability** of the seal component and the permeability of the DRZ surrounding that component; the effective permeability is calculated using the equations in Appendix PAR, Parameter 12. The effective permeability will decrease over time as the seal material consolidates and the DRZ heals; the values used in the performance assessment calculations reflect this process. For the crushed salt members of the seal system, salt consolidation over time is also expressed as a series of permeabilities which are used for the time periods under consideration. An **index** is employed in selecting the permeability for each time period to ensure that the modeled consolidation of the salt increases with time (and the resulting effective permeability decreases).

Additional material properties affect brine and gas flow through the seals: **residual brine saturation** (the minimum brine saturation at which liquid will flow), **residual gas saturation** (the minimum gas saturation at which gas flow will occur), and **pore shape distribution**. These parameters are representative of all the seal materials. The variations in reported values for the materials are incorporated into the performance assessment calculations through LHS.

### *MONPAR.3.10 Radionuclide Transport and Retardation*

*Radionuclides in dissolved and colloidal form may migrate from the repository into the Salado or into the Culebra through a borehole. The transport and retardation properties depend on the oxidation state and the form (dissolved or colloidal) of the actinide under consideration. The transport and retardation processes are significant to system performance and are incorporated into performance assessment.*

*Transport into the Salado or the Culebra will not occur during the active control period, thus monitoring in the operational or early postclosure periods will not provide useful information. In addition, it is not possible to monitor the Salado without jeopardizing the integrity of the disposal system. Therefore, transport in the Salado and the Culebra will not be monitored during the operational period nor during the postclosure period.*

Actinide transport in the Salado and the Culebra are considered to be possible mechanisms for release to the accessible environment. As in other areas of the disposal system, actinides may be transported as dissolved species or as colloidal particles. Actinide transport is affected by a variety of processes that may occur along the flow path.

Colloidal actinides are subject to retardation by chemical interaction between colloids and solid surfaces (represented by the **distribution coefficient ($K_d$)**) describing actinide partitioning or distribution between the solid and liquid phases) and by clogging of small pore throats (that is, filtration). However, colloidal particles, if not retarded, are transported slightly more rapidly than the average velocity of the bulk liquid flow. Because the effects are offsetting with respect to the potential for transport, residual effects of these opposing processes will be either small or beneficial. These effects are therefore not incorporated in the modeling of actinide transport in the Salado interbeds.

Radionuclides might be introduced into the Culebra by brine flowing up a borehole or by brine flowing up the DRZ around the shafts. However, modeling shows that the chief source of radionuclides in the Culebra is releases from an abandoned and unplugged borehole that intersects the repository. As noted in Section MONPAR.2.3, groundwater flow in the Culebra is described using a double-porosity model, in which a portion of the porosity is associated with high-permeability features where transport occurs by advection, and the rest of the porosity is associated with low-permeability features where flow does not occur.

Three principal processes affect the transport and retardation of dissolved actinides in the Culebra: (1) advection in the natural groundwater flow, (2) diffusion into the matrix, and (3) sorption to varying extents onto the minerals lining pore walls or fractures. Advection is the transport of contaminant with the bulk flow of liquid. Diffusion is the transport of contaminants due to molecular motion in the presence of concentration gradients. Dispersion is an additional component of transport of contaminant that occurs during liquid flow due to irregularities in the porous medium and differences in the velocity of liquid moving through pores. The sorption processes are incorporated into performance assessment models through a linear isotherm model expressing the concentration of actinide sorbed relative to the concentration of actinide in solution. The isotherms for sorption **in the Culebra** are represented by **distribution coefficients** ($K_d$) describing the distribution of each **dissolved actinide** in each oxidation state between the solid and liquid phases: Am(III), Pu(III), Pu(IV), U(IV), Th(IV), and U(VI).

Colloidal particles in the Culebra are subject to many of the same processes that affect dissolved actinides, but because of their size several additional processes affect them. There are three process differences. Colloidal particles in general are preferentially carried in the center of pore throats by faster-moving fluid located there, which causes slightly increased rates of transport. Colloidal particles can be restricted (filtered) from flowing groundwater when they encounter small-aperture features in the pore network. Finally, colloidal particles may undergo different sorption processes than dissolved species.

Actinide intrinsic colloids and humic materials are small enough for diffusion to occur, so the conceptual model for these **colloidal particles in the Culebra** is analogous to the model specified for dissolved actinides. The conceptual model assumes that other retardation processes (for example, filtration) will not occur.

In contrast, colloidal particles that are larger than pore throats in the matrix will be excluded from the matrix and will remain in advective porosity. Microbes and mineral fragments are larger than the mean pore-throat diameter; therefore the conceptual model for these particles includes the processes of advection and filtration by small-aperture features that occur within the advective porosity.

### MONPAR.4 Potentially Significant Parameters that Describe Human-Initiated Events and Processes

The parameters describing human-initiated events and processes that were considered in the analysis fall into five groups:

- Frequency of intrusion into the repository through drilling; this includes both the drilling rate and location of the drilling events.

- Consequences of future direct intrusion into the repository; direct releases in the form of cuttings, cavings, spallings, and direct brine flow to the surface during drilling.

- Properties of the boreholes that affect fluid flow and radionuclide transport, leading to long-term releases.

- Effects of current drilling and resource extraction activities (mining is treated separately) on groundwater flow in the vicinity of the disposal system.

- Effects of current and future mining in the McNutt potash zone in the Salado.

The results of DOE's analysis are presented in Table MONPAR-3. The parameters describing the human-initiated events and processes are discussed in the following section.

### *MONPAR.4.1 Drilling Intrusions*

*Intrusion into the repository through drilling may occur during the regulatory time period. In accordance with regulatory requirements, such intrusions are modeled to occur randomly in time and space. Drilling leads to direct releases during the drilling itself and possible long-term releases due to effects on fluid flow in the disposal system. The drilling rate (boreholes per square kilometer per 10,000 years) is significant to repository performance. The DOE uses a drilling rate in performance assessment that is based on historical rates in the Delaware Basin. The locations of the boreholes are also significant to performance assessment.*

*The DOE will monitor the drilling activity in the Delaware Basin during the operational and postclosure periods and will use the results in performance calculations performed in support of recertification.*

In keeping with the requirements of 40 CFR § 194.33(b)(1), the DOE models consequences of inadvertent human intrusion into the repository by drilling as the most severe scenario that may affect long-term performance of the disposal system. The DOE's treatment of the probability of inadvertent human intrusion is discussed in Section 6.4.12.2. Intrusions may occur at any time between 100 years and 10,000 years after final facility closure. The assumption that random drilling over the repository begins in 100 years after final facility closure is based on 100 percent effectiveness for the active institutional controls to be implemented by the DOE (Section 7.1 and Appendix AIC). The DOE's system of passive institutional controls will reduce the likelihood of intrusions for the next 600 years, but will not eliminate intrusions (See Section 2.3 and Appendix EPIC).

Both the number and time of intrusions are determined sequentially by sampling from a cumulative distribution function derived from the Poisson model that probabilistically describes the period that elapses between an intrusion and the next intrusion for a specified rate constant. The **time between intrusions**, or the time before the first intrusion, may vary from 0 years to greater than 9,900 years, with a probability determined by the rate constant $\lambda$. The rate constant is derived from the **drilling rate** established for the WIPP vicinity and the area of the repository. As discussed in Section 6.4.12.6 and Appendix DEL (Section DEL.7.4), this rate is based on a review of past and present drilling activity in the Delaware Basin. The rate constant is also time dependent in that while active institutional controls are 100 percent effective it is equal to zero, and while passive institutional controls are effective it is less than the uncontrolled drilling rate. The area corresponds to the total plan-view area of the waste-disposal region. Both the drilling rate and the time between intrusions are significant to performance assessment (See Appendix MASS).

## Table MONPAR-3. Potentially Signficant Human-Initiated Parameters

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Operational | Post-closure |
| Drilling intrusions | Intrusion into the repository | Intrusion boreholes provide pathways for fluid flow and radionuclide transport | Drilling rate | Performance assessment models and calculations | 1[c] | 1[c] | Y | Y |
| | | | Time between intrusions | | 1[c] | 1[c] | N | N |
| | | | *Borehole location* | | 1[c] | 1[c] | N | N |
| | | | Probability of encountering a brine reservoir in the Castile | | 1[c] | 1[c] | N | N |
| Direct releases | Direct releases from intrusion into the repository through future drilling. | Waste may be released by several mechanisms during drilling: cuttings, cavings, spallings, and brine blowout | Borehole diameter | Performance assessment models and *calculations* | 2[c] | 2[c] | N | N |
| | | | Waste activity | | 1[c] | 1[c] | Y | N |
| | | | Waste effective shear resistance to erosion | | 2[c] | 2[c] | N | N |
| | | | Waste particle diameter | | 1[c] | 1[c] | Y | N |
| | | | Waste tensile strength | | 2[c] | 2[c] | N | N |
| | | | Gravity factor for spalling | | 2[c] | 2[c] | N | N |
| | | | Strength factor for spalling | | 3 | 3 | N | N |
| Borehole properties | Properties of boreholes change over time | Borehole properties have long-term effects on fluid flow and radionuclide transport | Borehole permeability | Performance assessment models and calculations | 1[c] | 1[c] | Y | N |
| | | | Index for selecting type of borehole plug | | 1[c] | 1[c] | Y | N |

## Table MONPAR-3. Potentially Signficant Human-Initiated Parameters (Continued)

| Topic | Property or Process | Impact on Performance | Parameter(s) | Identification as a Potentially Significant Parameter | Significant Effects on Waste Containment[a] | Significant Effects on Verifying Predictions[a] | Retained for Monitoring[b] | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Operational | Post-closure |
| Human activity | Effects of current drilling and resource recovery activities. Ground water flow and other effects of human intrusion in the vicinity of the disposal system. | Groundwater flow is altered by current drilling and resource recovery activities. | Changes in groundwater flow in the Culebra (transmissivity, fracture and matrix porosity, fracture spacing and index, dispersivity)[d] | 40 CFR § 194.42(a)(4) | 2 | 2 | Y | N |
| | | | Changes in groundwater flow in the Salado (permeability, porosity, pore compressibility, model choice)[d] | | 3 | 3 | N | N |
| Mining | Effects of mining in the McNutt Potash Zone in the Salado. | Groundwater flow in the Culebra is altered by subsidence associated with potash mining activities. | Probability that mining will occur within a given century | Performance assessment models and calculations | 2 | 2 | N | N |
| | | | Mining index for adjusting Culebra transmissivity | | 2 | 2 | N | N |

[a] Significance legend: 1 - high, 2 - medium, 3 - low

[b] See Appendix MON for monitoring program.

[c] Significant only in intrusions: E1, E2, and E1E2. Significance is 3 in all other cases.

[d] The parameters listed in parentheses are among those used to calculate or model this property. Potentially significant parameters are also addressed separately.

Drilling events are assumed to be random in time and space, and the location of each intrusion borehole within the repository is sampled randomly. This is done in the analysis by discretizing a plan view of the area under the passive institutional control berms into 144 separate locations, and requiring each intruding borehole to penetrate one, and only one, location. The probability of intersecting each location is determined based on the fraction of the total plan-view area represented by the location.

The **location of an intrusion borehole** is used to determine whether a borehole that penetrates the repository intersects waste. Those boreholes that intersect the experimental and operational regions do not intersect waste and do not contribute to the direct releases at the ground surface during drilling. Intrusions into the experimental and operational regions may, however, contribute to long-term groundwater releases through the E1E2 scenario in which multiple wells penetrate the repository. Direct releases and long-term releases are discussed further in MONPAR.4.2 and MONPAR.4.3, respectively.

The **probability** of encountering a brine reservoir in the Castile is significant to long-term disposal system performance. Boreholes that intersect pressurized brine in the Castile below the repository are E1 events (Section 6.3.2.2.2), and boreholes that do not are E2 events (Section 6.3.2.2.1). Based on geophysical methods, geological structure analysis, and geostatistical correlation, the DOE has determined that there is an 8 percent probability that a reservoir will be encountered during any intrusion event (see Section 6.4.12.6).

### *MONPAR.4.2 Direct Releases*

The releases associated with direct intrusion into the repository are incorporated into performance assessment. These releases are significant to compliance, and are affected by conditions in the disposal area at the time of intrusion. The conceptual model includes assumptions about long-term performance (for example, waste properties after consolidation and degradation), and random events (such as drilling intrusions); these assumptions are not applicable during the preclosure period. The conceptual model also includes assumptions about long-term performance (for example, waste activity) that are applicable during the preclosure period.

*The waste in the closed repository will not achieve their long-term properties (consolidation, saturation) used in performance assessment during the operational period and for the first 100 years after closure. Therefore, long-term monitoring waste properties will not provide relevant information or verify assumptions used in performance assessment and need not be monitored.*

As discussed in Section 6.4.7.1, releases that may occur during and immediately following a drilling event are modeled under the assumption that future drilling practices will be the same as those of the present, consistent with the requirements of 40 CFR § 194.33(c)(1). If present day rotary drilling techniques are used to penetrate the waste, radionuclides may be brought to the surface by four means. First, some quantity of cuttings, which contain material intersected by the drill bit, will be brought to the surface by the drilling fluids. The release in this case is governed by the **activity of intersected waste** and the **diameter of the drill bit**.

Second, cavings, which contain material eroded from the borehole wall by the circulating drill fluid, may also be brought to the surface by the circulating drilling fluids. The release is affected by the **effective shear resistance to erosion**.

Third, if the repository contains fluids at pressures significantly higher than those anticipated by the driller for that depth, spalling of waste material into the borehole may occur as high-pressure gas flows into the borehole. Spalled material may be brought to the surface by continued drilling activity. The gas itself is not radioactive and will not contribute to the radionuclide release as it is vented at the surface. The **waste particle diameter** is significant for this release scenario. The **tensile strength** and **gravity factor** have a moderately significant effect on the quantity of material brought to the surface. The quantity is not significantly affected by the **strength factor**.

Fourth, brine as well as gas may enter the borehole from the repository if the driller is unable to control the pressure within the well or if the driller chooses not to control the pressure. The brine may flow to the surface, and if it has been in contact with waste, it may contain dissolved and/or suspended radionuclides. The properties of the Castile brine reservoir (MONPAR.2.5) are significant for this release. Properties of earlier intrusion boreholes (such as plug configurations and permeabilities) may affect conditions (such as pressure and fluid content) in the repository; these conditions in turn may affect the direct release of brine during drilling (borehole properties are discussed in MONPAR.4.3).

The geometry of the waste panels is represented in the model, and mathematical methods are applied to the conditions in the borehole to obtain accurate representation of the flow into the borehole (see Appendix MASS Section MASS.16 and Attachment 16-2). Hydrologic properties in the disposal room (MONPAR.3.4) have a moderately significant effect on performance assessment.

### *MONPAR.4.3 Borehole Properties*

*The properties of a borehole change over time, and are incorporated into performance assessment. The properties are established to be "consistent with practices in the Delaware Basin at the time a compliance application is prepared" [Part 194.33(c)(1)]. These parameters are significant to compliance.*

*The current practices will be monitored and changes will be incorporated into the performance assessment models of borehole properties in future calculations in support of recertification.*

Intrusion boreholes have long-term effects on fluid flow in the disposal system after the borehole casing and plugs installed at the time of abandonment have degraded. The presence of the degraded borehole may provide a pathway for fluid flow between the repository and the surrounding formations, and for radionuclide migration toward the accessible environment.

The fluid flow between the repository and surrounding formations (particularly a brine reservoir in the Castile) may affect conditions (such as pressure and fluid content) within the repository; these conditions could in turn affect direct releases during drilling (MONPAR.4.2).

Borehole plug configurations used today in the Delaware Basin vary based on the local stratigraphy encountered in the hole, its total depth, and the types of fluids present. Each of these plugging configurations meets the minimum requirements of the applicable plugging regulations. All holes are plugged with some combination of solid concrete plugs isolating different fluid-bearing horizons from each other and from the ground surface. As discussed in detail in Appendix DEL Section DEL.5, six different plug configurations are identified that are potentially relevant to future borehole abandonment practice at the WIPP. As discussed in Appendix MASS Section MASS.16.3.3, these six plug configurations can be approximated for performance assessment by three conceptual plugging patterns. Probabilities of occurrence for each of these three plugging configurations are discussed in Section 6.4.12.7.

The first type of plug incorporated in the performance assessment models is the continuous concrete plug described in Section 6.4.7.2.1. Because of the small cross-sectional area and low permeability of the potential pathway, long-term releases through this plug are assumed to be zero.

In the two-plug configuration, two concrete plugs are assumed to have a significant effect on long-term flow in the borehole. These plugs initially have the properties of intact concrete. The lower plug of interest is assumed to be located somewhere between the hypothetical Castile brine reservoir and underlying formations. A second plug is located within the lower portion of the Rustler Formation, immediately above the Salado. As described in Section 6.4.7.2.2, the steel casing in the borehole and the upper concrete plug are assumed to have failed completely after 200 years, and the borehole is filled with a silty-sand-like material composed of degraded concrete, corrosion products, and material that sloughs from the borehole walls. The plug below the Castile brine reservoir is located in a less aggressive chemical environment, and its properties remain constant in performance assessment. The permeability in the borehole between the repository and the Castile is modeled assuming a decrease after 1,000 years as creep closure consolidates the material in the borehole. The borehole does not close completely in 10,000 years.

In the three-plug configuration (Section 6.4.7.2.3), three concrete plugs are assumed to have an effect on long-term flow in the borehole. Again, the plugs initially have the properties of intact concrete. Two of the plugs are identical to those modeled in the two-plug configuration. The third plug is located within the Castile above the brine reservoir and below the waste-disposal panel. This plug is assumed to behave in the same manner as the lower plug in the two-plug configuration: that is, its properties remain unchanged in performance assessment. Otherwise, all portions of the borehole in the three-plug configuration are assumed to have the same material properties as the corresponding regions in the two-plug configuration, with adjustments to borehole-fill permeability occurring 1,000 years after failure of the overlying plug.

The DOE has chosen not to model this configuration explicitly in the performance assessment calculations, as the boreholes in which the three-plug configuration is emplaced are assumed to result in long-term releases comparable to those calculated for E2 intrusions, regardless of whether they penetrate a Castile brine reservoir.

The **permeability** of the borehole is varied to represent degradation of the two-plug and three-plug configurations after 200 years and the resulting increase in permeability. The **plug index** is used to represent the probability that the borehole under consideration has a continuous two-plug or three-plug configuration.

### *MONPAR.4.4 Current Drilling and Resource Recovery*

*Historical, current and near-future human activities in the vicinity of the repository could affect groundwater flow in the Culebra prior to closure of the repository, as well as subsequent to repository closure. The significance of these human activities depends on the extent and magnitude of the induced hydrological, geochemical and mechanical disturbance. Changes in groundwater in the Culebra are moderately significant to performance. Such changes are incorporated into performance assessment as described in MONPAR.4.5. Changes in brine flow in the Salado as a result of any current or near-future human activities in the vicinity of the repository is not anticipated and therefore are not significant to performance assessment.*

*The DOE will monitor water levels in the Culebra during the operational period to detect deviations from expected performance. Monitoring of groundwater flow conditions in the Salado could create additional pathways for radionuclide transport, and would potentially jeopardize long-term performance of the disposal system; thus the DOE will not perform such monitoring.*

Historical, current and near-future human activities outside the controlled area could affect groundwater flow and chemistry conditions and other properties of the disposal system. A potentially significant effect of human activities will be to alter hydrological conditions in the Culebra significantly, which, in the event of radionuclide migration to the Culebra, could result in altered travel times for radionuclide transport to the accessible environment (Sandia National Laboratories 1992).

Activities that could impact the long-term performance of the disposal system that are currently taking place and expected to continue in the near future outside the controlled area are:

- Drilling associated with water, potash, oil, and gas exploration and production,

- Water, oil, and gas production, and

- Disposal of liquid by-products from oil and gas production.

The effects of historical, current, and near-future drilling, activities involving the use of a borehole (fluid extraction or injection), and flow through abandoned boreholes have been eliminated from performance assessment calculations on the basis of low consequence to the performance of the disposal system.

Groundwater flow conditions in the Culebra will affect containment of waste in the disposal system in the event of radionuclide migration to the Culebra. Furthermore, subsidence due to potash mining in the vicinity of the WIPP (MONPAR.4.5) may lead to **changes in groundwater flow in the Culebra**. Thus, water levels in the Culebra will be monitored in the preclosure period to build confidence in Culebra groundwater conditions (see Appendix GWMP).

**Groundwater flow in the Salado** is not expected to change as a result of any current or near-future human activities (other than activities associated with operation of the repository). Monitoring of groundwater flow conditions in the Salado could create additional pathways for radionuclide transport, and would potentially jeopardize long-term performance of the disposal system. Therefore, no monitoring of Salado groundwater flow will be conducted.

### *MONPAR.4.5 Mining*

*The McNutt in the Salado is present in the controlled area overlying the repository. The probability that the potash will be mined and the effects on system performance are incorporated into performance assessment in accordance with the conceptual model in Parts 194.32(b) and (c). The effects are moderately significant to long-term disposal system performance. Monitoring the effects of human activities in the vicinity of the WIPP is discussed in MONPAR.4.4.*

The only natural resource being mined currently near the WIPP is potash from the McNutt zone of the Salado, and it is the only mineral considered for future mining. Mineral resources within the disposal system that are similar in quality and type to those currently being mined outside the controlled area are assumed to be mined at an uncertain time in the future. Outside the disposal system, mineral resources reasonably expected to be mined in the near future are also assumed to be mined. These effects are included in analyses of both disturbed and undisturbed performance. Inside the disposal system, **whether a mining event occurs in any given century** after the active institutional control period is determined by a probabilistic model. Outside the disposal system, what is reasonably expected to be mined is assumed to be mined by the end of WIPP disposal operations. With respect to consequence analysis, mining affects only the hydraulic conductivity of the units overlying the Salado as discussed in Section 6.4.6.2.3.

The DOE has identified areas that are assumed to be mined in a manner consistent with the conceptual model and other guidance presented by the EPA in Part 194. Appendix MASS

(Section MASS.15.4 and Attachments MASS 15.4 and MASS 15.5) includes a description of the method used to determine the extent of mining in the McNutt both inside and outside the disposal system. The changes in hydraulic conductivity due to mining inside and outside of the controlled area are modeled in performance assessment as changes in the Culebra transmissivity due to subsidence induced by the excavated potash. The transmissivity changes are executed through a **mining index** used to uniformly adjust the transmissivity of the affected areas by a factor between 1 and 1,000 that is randomly sampled in LHS.

The effects of mining all potash deposits "similar in quality and type to those resources currently extracted from the Delaware Basin" (40 CFR § 194.32[b]) outside the disposal system are included in the undisturbed performance scenario, and are therefore included in all scenarios. In other words, all calculations of transport in the Culebra include the effects of mining outside the controlled area. This is the undisturbed mining case because mining within the disposal system has not occurred.

If mining occurs within the disposal system, an area of the Culebra inside and outside the disposal system will be affected. This is the disturbed mining case. To evaluate the impact of disturbed mining, a second simulation of Culebra flow directions and rates is executed on both the regional and local domains. In this second simulation, the location-specific values in the transmissivity field are multiplied by the same mining multiplier used for the undisturbed mining case.

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# MONPAR ATTACHMENT A

**Sandia National Laboratories**

Albuquerque, New Mexico 87185-1341

date: August 20, 1996

to: Distribution

IP T.W. Hicks Yifeng Wang T.W. Hicks

from: David Bennett, Yifeng Wang, and Tim Hicks

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subject: An Evaluation of Heat Generation Processes for the WIPP

## 1.0 Introduction

Nuclear criticality, exothermic reactions, and radioactive decay are possible sources of heat in the WIPP repository. Nuclear criticality has been eliminated from performance assessment calculations on the basis of low probability (see SNL Summary Memo of Record RNT-1). This memo discusses possible heat generating processes at the WIPP and the potential magnitude of the temperature increases they might induce. Heat from exothermic reactions is discussed in Section 2 and heat from radioactive decay is discussed in Section 3.

Conclusions are provided in Section 4. In summary, soon after disposal concrete hydration in the panel closures and shaft seals will give rise to temperature increases lasting a few decades. Heat from radioactive decay will generate a maximum temperature increase of less than 2°C above the ambient temperature (about 27°C) within 100 years after disposal. A number of potential exothermic reactions other than concrete hydration have been identified. These reactions are brine limited and will cause only minor perturbations to the temperature distribution within the disposal system. The maximum calculated rate of brine inflow to a waste disposal panel, and thus, the maximum exothermic reaction rates, occur for the S2 scenario involving an E1 drilling event at 350 years after disposal. By the time such a drilling event takes place heat generation from concrete seal hydration and radioactive decay will have decreased substantially, and the temperatures in the disposal rooms will have reduced to close to initial values. Note that active institutional controls are expected to prevent drilling within the controlled area for 100 years after disposal. Thus, exothermic reactions following a drilling intrusion into a waste disposal panel will be the only potentially significant heat generating processes at the time of a drilling intrusion.

The maximum temperature that could be achieved in the panel following a drilling intrusion at 350 years occurs as a result of aluminum corrosion; this reaction could result in a maximum temperature increase of about 6°C two years after the drilling event. This predicted value of temperature increase is based on several conservative assumptions. For example, it is assumed that no aluminum corrosion has occurred prior to the drilling event and that all the brine introduced to the waste panel is available for aluminum corrosion. In reality some aluminum corrosion is likely to have occurred prior to the drilling event, reducing the volume of aluminum available for the reaction, and other reactions with lower reaction enthalpies (such as backfill hydration) or lower reaction rates (such as microbial degradation) will compete with aluminum corrosion to consume brine resulting in a smaller temperature increase. Based on similar conservative assumptions, backfill hydration could result in a maximum temperature increase of less than 5°C. These maximum heat generation rates resulting from aluminum corrosion and backfill hydration could not occur simultaneously because they are limited by brine availability. Thus, the temperature rise of 6°C represents the maximum that could occur as a result of any combination of exothermic reactions occurring simultaneously.

## 2.0 Heat From Exothermic Reactions

Exothermic reactions in the repository will liberate heat resulting in elevated temperatures. The magnitude and duration of this temperature increase will depend on the amount and rate of energy release, the geometry of the heat source, the thermal conductivities of the surrounding rocks, and any influence of groundwater or brine flow on heat transport.

In the WIPP a range of different types of reactions will occur, including corrosion, microbial degradation, waste dissolution, and concrete and backfill hydration, and these will liberate different amounts of heat at different times. The amount of heat liberated by the different reactions will depend on the extent of reaction that occurs (for example, how much gas generation or concrete hydration takes place), and the enthalpy of the reactions. The former will depend on the inventory of materials emplaced in the WIPP, and the subsequent chemical evolution of the repository system. The latter can be assessed by considering typical enthalpies for the reaction types of interest.

Enthalpies of reaction, $\Delta_r H^\circ$, for example reactions representing processes that may take place in the repository are given in Table 1 (from SNL Summary Memo of Record GG-7, SP-7). The reactions shown are based on the chemical conditions expected in the WIPP. Note that negative values for $\Delta_r H^\circ$ indicate that the reactions liberate heat as they progress from left to right.

Table 1. Enthalpies of reaction, $\Delta_r H°$, for the WIPP

| Reaction | Example Stoichiometry and Standard Enthalpies of Formation, $\Delta_f H°$ (kJ/mol) | Reaction Enthalpy $\Delta_r H°$ (kJ/mol) | Data Source |
|---|---|---|---|
| Backfill hydration | $MgO_{(s)} + H_2O_{(l)} = Mg(OH)_{2(s)}$<br>$\Delta_f H°$ -601.7 -285.8 -925.5 | -38 | Krauskopf, 1982, 561 |
| Backfill carbonation | $Mg(OH)_2 + CO_2(g) = MgCO_3 + H_2O$<br>$\Delta_f H°$ -925.4 -393.1 -1110.3 -285.8 | -77 | Drever, 1982, 351-256 |
| Microbial degradation | $C_6H_{10}O_5 + H_2O = 3CH_4 + 3CO_2$<br>$\Delta_f H°$ -805.5 -285.8 3 x (-74.4) 3x (-393.5) | -312 | Lide, 1994, 5-16 to 5-37 |
| Aluminum Corrosion | $Al + 3H_2O = Al(OH)_3 + 1.5H_2$<br>$\Delta_f H°$ 0 3x(-285.8) 1291.9 0 | -434 | Drever, 1982, 351-256 |
| Anoxic corrosion of steel | $Fe_{(s)} + 2H_2O_{(l)} = Fe(OH)_{2(s)} + H_{2(g)}$<br>$\Delta_f H°$ 0 2 x (-285.8) -569.0 0 | +2.7 | Wagman et al., 1982, Table 41 |
| Waste dissolution | $UO_{2(s,cr)} + 2H_2O_{(l)} = U(OH)_{4(aq)}$<br>$\Delta_f H°$ -1085.0 2 x (-285.8) -1655.8 | +0.9 | Grenthe et al., 1992, Table III-1 |
| Concrete hydration | $CaO_{(s)} + H_2O_{(l)} = Ca(OH)_{2(s)}$<br>$\Delta_f H°$ -635.1 -285.8 -986.1 | -65.2 | Wagman et al., 1982, 2-26 |

Even though there is uncertainty surrounding the extent of reactions that will occur, the reaction enthalpies indicate that the thermal effects of anoxic corrosion of steel and the waste dissolution reaction will be endothermic and will be of low consequence to the performance of the disposal system. However, the other reactions shown in Table 1 have the potential to evolve significant amounts of heat. The potential effects of these processes on the temperature within the disposal system are discussed below.

## 2.1 Backfill Hydration

Potential temperature increases in the repository as a result of exothermic backfill hydration reactions have been evaluated by Wang (1996, attachment to this memo). In his analysis, Wang (1996) made the following assumptions:

- The reaction will proceed rapidly so that the rate of heat generation will be controlled by brine availability.

- All brine entering a waste disposal panel will contact and react with the backfill in the panel uniformly.
- All of the emplaced backfill will undergo hydration.

The maximum calculated rate of brine inflow into a panel (about 200 $m^3$/year) occurs for the S2 scenario involving an E1 drilling event at 350 years after disposal. The molar density of water is $5.56 \times 10^4$ moles/$m^3$, and thus, the reaction rate of backfill hydration in the panel will be $1.1 \times 10^7$ moles/year. Based on the reaction enthalpy shown in Table 1, backfill hydration will generate a thermal load of about 13 kW. There will be about $2 \times 10^8$ moles MgO emplaced per panel and thus the reaction could continue for about 20 years if sufficient brine was available.

Wang (1996) estimated the maximum temperature that could be generated by backfill hydration within a panel. Assuming heat loss will occur by conduction through the salt forming the roof and floor of the panel and that heat losses through the side walls are negligible, Wang (1996) calculated that the maximum temperature rise in a panel, as a consequence of backfill hydration following a borehole intrusion and subsequent brine inflow, would be about 4.5°C.

### 2.2 Backfill Carbonation

Wang (1996) also estimated the potential temperature rise that could occur as a result of backfill carbonation. Wang (1996) assumed that the reaction will be limited by microbial $CO_2$ production; the maximum rate of $CO_2$ production is $2.9 \times 10^5$ moles/year. Based on the reaction enthalpy shown in Table 1, backfill carbonation will generate a thermal load of about 0.7 kW. About $3.6 \times 10^7$ moles $CO_2$ could be produced in a single panel (see Wang, 1996) and thus the reaction could continue for about 125 years. Wang (1996) estimated the maximum temperature that could be generated by backfill carbonation within a panel to be about 0.6°C.

### 2.3 Microbial Degradation

Wang (1996) estimated the maximum reaction rate for microbial degradation in a panel to be about $1 \times 10^5$ moles/year and the inventory to be about $1.2 \times 10^7$ moles $C_6H_{10}O_5$ per panel. Thus, the reaction could continue for about 120 years. Based on the reaction enthalpy shown in Table 1, microbial degradation will generate a thermal load of about 1 kW. Wang (1996) estimated the maximum temperature that could be generated by microbial degradation within a panel to be about 0.8°C.

### 2.4 Aluminum Corrosion

Wang (1996) determined that the rate of corrosion of aluminum will be controlled by brine availability. From Table 1, the reaction rate of aluminum corrosion in the panel will be about $0.4 \times 10^7$ moles/year, assuming a brine inflow rate of 200 $m^3$/year ($1.1 \times 10^7$ moles/year). About $8 \times 10^6$ moles of aluminum will be emplaced in each panel and thus aluminum corrosion could continue for 2 years. Based on the reaction enthalpy shown in Table 1, aluminum corrosion will generate a thermal load of about 51 kW. Wang (1996) estimated the maximum temperature that could be generated by aluminum corrosion within a panel to be about 6°C.

### 2.5 Concrete Hydration

Concrete hydration reactions will occur in the seals and panel closures and in the waste.

#### 2.5.1 Seals and panel closures

Concrete hydration reactions are known to proceed for extended periods (perhaps thousands of years). However, the rates of these reactions decrease with time and, within the WIPP, the greatest evolution of heat will occur during the short periods following emplacement of panel closures during the operational phase and following shaft seal emplacement and repository closure. A quantitative analysis of the thermal effects of emplacing large concrete seals in salt at the WIPP was made by Loken (1994), Loken and Chen (1995). Their analysis showed that the energy released by the hydration of the seal concrete could raise the temperature of the concrete to approximately 53° C and that of the surrounding salt to approximately 38° C one week after seal emplacement.

#### 2.5.2 Waste

WIPP waste contains cement which is used to solidify liquids, particulates and sludges. Storz (1996) estimated that all the waste to be emplaced at the WIPP will contain a total of about $8.5 \times 10^6$ kg of cement. This is equivalent to about $1.5 \times 10^7$ moles of calcium oxide (CaO) per waste disposal panel, representing the cement as CaO. Although a substantial amount of hydration may occur prior to waste disposal, this process will continue at a slower rate after disposal. Disregarding the hydration that will occur prior to disposal and assuming a brine inflow rate of 200 $m^3$/year, the reaction rate of concrete hydration in the panel will be about $1.1 \times 10^7$ moles/year, and the reaction could continue for about 1.4 years. Based on the reaction enthalpy shown in Table 1, concrete hydration will generate a thermal load of about 23 kW. Thus, using analyses similar to that used by Wang (1996) the maximum temperature that could be generated by concrete hydration of the waste within a panel is about 2°C.

## 3.0 Heat From Radioactive Decay

Radioactive decay of the contact handled CH and remote handled RH TRU waste emplaced in the repository will generate heat. The importance of heat from radioactive decay depends on the effects that the induced temperature changes would have on mechanics, fluid flow, and geochemical processes. For example, temperature increases could result in thermally induced fracturing, regional uplift, or thermally driven flow of gas and brine in the vicinity of the repository.

According to the Waste Acceptance Criteria (WAC), the design basis for the WIPP requires that the thermal loading does not exceed 10 kilowatts per acre. The WAC also require that the thermal power generated by waste in an RH TRU container shall not exceed 300 watts, but the WAC do not limit the thermal power of CH TRU waste containers.

A numerical study to calculate induced temperature distributions and regional uplift is reported in DOE (1980, pp.9-149–9-150). This study involved estimation of the thermal power of CH TRU waste containers. The DOE (1980) analysis assumed:

- All CH TRU waste drums and boxes contain the maximum permissible quantity of plutonium. According to the WAC, the fissionable radionuclide content for CH TRU waste containers shall be no greater than 200 grams per 0.21 cubic meter drum and 350 grams per 1.8 cubic meter standard waste box (in Pu-239 fissile gram equivalents).

- The plutonium in CH TRU waste containers is weapons grade material producing heat at 0.0024 watts per gram. Thus, the thermal power of a drum is approximately 0.5 watts and that of a box is approximately 0.8 watts.

- Approximately $3.7\times10^5$ cubic meters of CH TRU waste are distributed within a repository enclosing an area of $7.3\times10^5$ square meters. This is a conservative assumption in terms of quantity and density of waste within the repository, because the maximum capacity of the WIPP is $1.756\times10^5$ cubic meters for all waste (as specified by the Land Withdrawal Act [LWA]) to be placed in an enclosed area of approximately $5.1\times10^5$ square meters.

- Half of the CH TRU waste volume is placed in drums and half in boxes so that the repository will contain approximately $9\times10^5$ drums and $10^5$ boxes. Thus, a calculated thermal power of 2.8 kilowatts per acre (0.7 watts per square meter) of heat is generated by the CH TRU waste.

- Insufficient RH TRU waste is emplaced in the repository to influence the total thermal load.

Thorne and Rudeen (1980) estimated the long-term temperature response of the disposal system to waste emplacement. Calculations assumed a uniform initial power density of 2.8 kilowatts per acre (0.7 watts per square meter) which decreases over time. Thorne and Rudeen (1980) attributed this thermal load to RH TRU waste, but DOE (1980), more appropriately, attributed this thermal load to CH TRU waste based on the assumptions listed above. Thorne and Rudeen (1980) estimated the maximum rise in temperature at the center of a repository to be 1.6°C at 80 years after waste emplacement.

Sanchez and Trellue (1996) estimated the maximum thermal power of an RH TRU waste container. The Sanchez and Trellue (1996) analysis involved inverse shielding calculations to evaluate the thermal power of an RH TRU container corresponding to the maximum permissible surface dose; according to the WAC the maximum allowable surface dose equivalent for RH TRU containers is 1000 rem/hr. The following calculational steps were taken in the Sanchez and Trellue (1996) analysis:

- Calculate the absorbed dose rate for gamma-ray radiation corresponding to the maximum surface dose equivalent rate of 1000 rem/hr. Beta and alpha radiation are not included in this calculation because such particles will not penetrate the waste matrix or the container in significant quantities. Neutrons are not included in the analysis because, according to the WAC, the maximum dose rate from neutrons is 270 mrem/hr, and the corresponding neutron heating rate will be insignificant.

- Calculate the exposure rate for gamma radiation corresponding to the absorbed dose rate for gamma radiation.

- Calculate the gamma flux density at the surface of a RH TRU container corresponding to the exposure rate for gamma radiation. Assuming the gamma energy is 1.0 MeV the maximum allowable gamma flux density at the surface of a RH TRU container is about $5.8 \times 10^8$ gamma rays per square centimeter per second.

- Determine the distributed gamma source strength, or gamma activity, in an RH container from the surface gamma flux density. The source is assumed to be shielded such that the gamma flux is attenuated by the container and by absorbing material in the container. The level of shielding depends on the matrix density. Scattering of the gamma flux, with loss of energy, is also accounted for in this calculation through inclusion of a gamma buildup factor.

The distributed gamma source strength is determined assuming a uniform source in a right cylindrical container. The maximum total gamma source (gamma curies) is then calculated for a RH TRU container containing 0.89 cubic meters of waste. For the waste of greatest expected density (about 6,000 kilograms per cubic meter) the gamma source is about $2 \times 10^4$ curies per cubic meter.

- Calculate the total curie load of a RH TRU container (including alpha and beta radiation) from the gamma load. The ratio of the total curie load to the gamma curie load was estimated through examination of the radionuclide inventory presented in the WIPP Baseline Inventory Report (BIR) (DOE, 1995). The gamma curie load and the total curie load for each radionuclide listed in the WIPP BIR were summed. Based on these summed loads the ratio of total curie load to gamma curie load of RH TRU waste was calculated to be 1.01.

- Calculate the thermal load of a RH TRU container from the total curie load. The ratio of thermal load to curie load was estimated through examination of the radionuclide inventory presented in the WIPP BIR (DOE, 1995). The thermal load and the total curie load for each radionuclide listed in the WIPP BIR were summed. Based on these summed loads the ratio of thermal load to curie load of RH TRU waste was calculated to be about 0.0037 watts/curie. For a gamma source of $2 \times 10^4$ curies per cubic meter the maximum permissible thermal load of a RH TRU container is about 70 watts per cubic meter. Thus, the maximum thermal load of a RH TRU container is about 60 watts, and the WAC upper limit of 300 watts will not be achieved.

Note that Sanchez and Trellue (1996) calculated the average thermal load for a RH TRU container to be less than 1 watt. Also, the total RH TRU heat load is less than 10% of the total heat load in the WIPP. Thus, the total thermal load of the RH TRU waste will not significantly affect the average rise in temperature in the repository resulting from decay of CH TRU waste.

Temperature increases will be greater at locations where the thermal power of a RH TRU container is 60 watts, if any such containers are emplaced. Sanchez and Trellue (1996) estimated the temperature increase at the surface of a 60 watt RH TRU waste container. Their analysis involved solution of a steady-state thermal conduction problem with a constant heat source term of 70 watts per cubic meter. These conditions represent conservative assumptions because the thermal load will decrease with time as the radioactive waste decays. The temperature increase at the surface of the container was calculated to be about 3°C.

In summary, analysis has shown that the average temperature increase in the WIPP repository due to radioactive decay of the emplaced CH and RH TRU waste will be about 1.6°C, with a maximum rise occurring at the center of the repository at about 80 years after waste emplacement. Temperature increases of about 3°C may occur in the vicinity of RH TRU containers with the highest allowable thermal load of about 60 watts (based on the maximum allowable surface dose equivalent for RH TRU containers).

## 4.0 Conclusions

Heat from exothermic reactions and radioactive decay will result in minor temperature increases in the repository. The potential temperature increases caused by these processes are summarized in Table 2.

Table 2. Maximum temperature increases at the WIPP.

| Heat Source | Maximum temperature increase | Time of maximum temperature increase |
|---|---|---|
| Backfill hydration | 4.5°C | 20 years after a drilling intrusion |
| Backfill carbonation | 0.6°C | 125 years after a drilling intrusion |
| Microbial degradation | 0.8°C | 120 years after a drilling intrusion |
| Aluminum corrosion | 6.0°C | 2 years after a drilling intrusion |
| Concrete hydration (seals) | 25°C in the shaft seal<br>10°C in the surrounding salt | 1 week after emplacement |
| Concrete hydration (waste) | 2.0°C | 1.4 years after a drilling intrusion |
| Radioactive decay of CH TRU waste | 1.6°C | 80 years after disposal |
| Radioactive decay of RH TRU waste | 3°C near a few containers | Within 100 years after disposal |

During the operational phase and soon after disposal concrete hydration in the panel closures and shaft seals will give rise to temperature increases lasting a few decades. Heat from radioactive decay will generate a maximum temperature increase of less than 2°C within 100 years after disposal. A number of potential exothermic reactions have been identified. These reactions are brine limited and will cause only minor perturbations to the temperature distribution within the disposal system. The maximum calculated rate of brine inflow to a waste disposal panel occurs for the S2 scenario involving an E1 drilling event at 350 years after disposal. The maximum temperature that could be achieved in the panel occurs as a result of aluminum corrosion; this reaction could result in a maximum temperature increase of about 6°C two years after the drilling event. Similarly, rapid backfill hydration could result in a maximum temperature increase of less than 5°C. These predicted values of temperature increase are based on a number of conservative assumptions. For example, the calculated temperature resulting from aluminum corrosion is based on the assumption that no corrosion has occurred prior to the drilling event and that all the brine introduced to the waste panel is available for aluminum corrosion. In reality some aluminum corrosion is likely to have occurred prior to the drilling event, reducing the volume of aluminum available for the reaction, and other reactions with lower reaction enthalpies or lower reaction rates will consume brine resulting in a smaller temperature increase.

Temperature increases of the magnitude and duration shown in Table 2 will have no significant effects on the performance of the disposal system. The effects of such temperature increases on the performance of the disposal system have been discussed in the SNL Summary Memos of Record RNT-24 (thermochemical effects), S-10 and GG-4 (thermal convection), S-11, SP-6, RM-1 (thermally-induced stress).

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Attachment: memorandum of August 19, 1996, by Yifeng Wang, to Distribution. "Evaluation of the Thermal Effect of Exothermal Chemical Reactions for WIPP Performance Assessment: A revised version," Sandia National Laboratories.

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Albuquerque, New Mexico 87185-1341

date: August 19, 1996

to: Distribution

from: Yifeng Wang (Org. 6832)

subject: Evaluation of the Thermal Effect of Exothermal Chemical Reactions for WIPP Performance Assessment: A revised version

Temperature increases caused by exothermal chemical reactions in the repository have been evaluated in the memo by Wang (1996). This memo is the revised version of the previous memo. Two revisions have been made: (1) anoxic steel corrosion reaction is no longer an exothermal reaction; (2) waste panel number is adjusted from eight to ten. All revisions made here do not change the conclusion that the thermal effect of exothermal chemical reactions in the repository is negligible.

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**Assumptions:**

The following exothermal chemical reactions are considered:

$$MgO + H_2O \rightarrow Mg(OH)_2 \quad (1)$$

$$Mg(OH)_2 + CO_2 \rightarrow MgCO_3 \quad (2)$$

$$C_6H_{10}O_5 + H_2O \rightarrow 3CH_4 + 3CO_2 \quad (3)$$

$$Al + 3H_2O \rightarrow Al(OH)_3 + 1.5\ H_2\,. \quad (4)$$

Anoxic steel corrosion is a major chemical reaction expected to occur in the repository:

$$Fe + 2H_2O \rightarrow Fe(OH)_2 + H_2. \quad (5)$$

However, this reaction is considered here, because it is not an exothermal reaction. The enthalpy change of Reaction (5) is estimated to be 0.64 Kcal/mole Fe.

Considering that the vertical dimension of the repository (~ 1 m, B. M. Butcher, personal comm.) will be much less than the horizontal extension after room closure, we assume that the heat released from the reactions will be dissipated away mainly from the ceiling and ground of the repository and the heat loss from the side walls is negligible. We also assume that all reactions will take place uniformly in a reaction region of interest. We here restrict the reaction region in a single waste panel, for the following reason: Some of the above reactions may be limited by brine inflow. BRAGFLO simulations have shown that, in the human intrusion cases, the rate of brine inflow into a borehole-penetrated waste panel will be significantly higher than that into the rest of the repository. Choosing a panel rather than the whole repository as a reaction region will make heat generation rate per unit of volume higher and the heat dissipating surface area smaller in our calculations, and therefore it is conservative. However, this choice will not affect the calculations for the reactions that are not limited by brine inflow, as you will see below.

**Theory:**

Based on these assumptions, the thermal effect of an exothermal chemical reaction can be modeled by a simplified system shown in Figure 1. The temperature distribution (T) can be described by the following equations:

$$C_p \rho \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial X^2} \qquad (6)$$

$$T(X,0) = T_0 \qquad (7)$$

$$R \Delta H = 2Sk \left. \frac{\partial T}{\partial X} \right|_{X=0} \qquad (8)$$

$$T(\infty,t) = T_0 \qquad (9)$$

where $C_p$ is the heat capacity of surrounding rocks (J/mole/K); $\rho$ is the molar density of surrounding rocks (moles/$m^3$); t is time (year); X is the spatial coordinate (m); k is the thermal conductivity of surrounding rocks (J/year/m/K); $T_0$ is the background temperature (K); R is the reaction rate (moles/year); $\Delta H$ is the enthalpy change of the reaction (J/mole); S is the horizontal area of a waste panel ($m^2$).

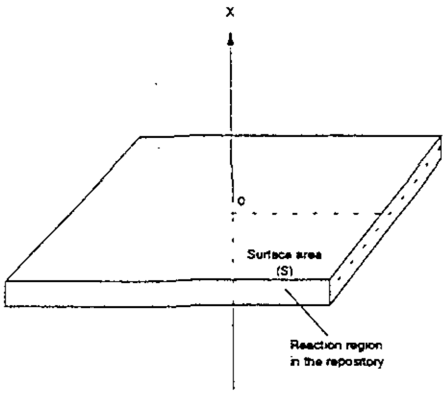


Figure 1. A modeling system for heat production and conduction.

The above equations can be solved for T with a Laplace-transformation method:

$$T - T_0 = -\frac{R\Delta H}{2S\sqrt{C_p\rho k}}\left[2\sqrt{\frac{t}{\pi}}e^{-\frac{C_p\rho X^2}{4Kt}} - \sqrt{\frac{C_p\rho}{k}}X\,erfc\left(\frac{X}{2}\sqrt{\frac{Cp\rho}{kt}}\right)\right]. \qquad (10)$$

The temperature increase in the repository ($\Delta T$) is obtained by setting $X = 0$ in equation (6):

$$\Delta T = T(0,t) - T_0 = -\frac{R\Delta H}{S}\sqrt{\frac{t}{\pi C_p\rho k}}. \qquad (11)$$

Equation (7) shows that the repository temperature will increase with t until $t = \frac{M}{R}$, when all the reactant is consumed. Here M is the inventory of the reactant in a waste panel (moles). Therefore, the maximum temperature increase ($\Delta T_{max}$) in the repository due to the exothermal reaction can be calculated by

$$\Delta T_{max} = T(0,t) - T_0 = -\frac{\Delta H}{S}\sqrt{\frac{RM}{\pi C_p\rho k}}. \qquad (12)$$

Equation (12) shows that, for the reactions not limited by brine inflow, reducing the reaction region size does not affect $\Delta T_{max}$, because the parameters S, R, and M will be reduced by the same factor, which is canceled out in the equation. This is not true for the brine-limited reactions, the rates of which are no longer dependent on reactant inventory.

Assuming the physical properties of the surrounding rocks can be represented by halite, we then have:

$C_p = 50$ J/mole/K (Lide, 1994, p. 12-158)
$\rho = 3.7\text{x}10^4$ moles/m$^3$ (Lide, 1994, p. 4-149)
$k = 6$ W/m/K $= 1.9\text{x}10^8$ J/year/m/K (Lide, 1994, p. 12-165)
$S = 1.2\text{x}10^4$ m$^2$ (Sandia WIPP Project, 1992, p. 3-4).

With these parameter values, we obtain from equation (12):

$$\Delta T_{max} = 2.5x10^{-12} \Delta H \sqrt{RM} \; . \qquad (13)$$

**Results:**

*(1) Reaction:* $MgO + H_2O \rightarrow Mg(OH)_2$

We assume that this reaction is instantaneous and thus is limited by brine inflow. Based on BRAGFLO simulations for E1 scenario (Figure 2), the conservative (maximum) estimate of the rate of brine inflow into a borehole penetrated waste panel is about 200 $m^3$/year, equivalent to the reaction rate of $1.1x10^7$ moles/year. With $\Delta H = -3.9x10^4$ J/mole (Drever, 1982, p. 351-356) and $M = 2x10^8$ moles, we estimate $\Delta T_{max}$, ≈ 4.5 K.

*(2) Reaction:* $Mg(OH)_2 + CO_2(g) = MgCO_3 + H_2O$

We assume that this reaction is limited by microbial $CO_2$ production. It is estimated that the maximum rate of $CO_2$ production (R) is $2.9x10^5$ moles/year and the total $CO_2$ that can be produced (M) is $3.6x10^7$ moles in a single waste panel (Wang & Brush, 1996; DOE/CAO, 1996). With $\Delta H = -0.8x10^5$ J/mole (Drever, 1982, p. 351-256), $\Delta T_{max}$, is estimated to be 0.6 K.

*(3) Microbial degradation:* $C_6H_{10}O_5 + H_2O \rightarrow 3CH_4 + 3CO_2$

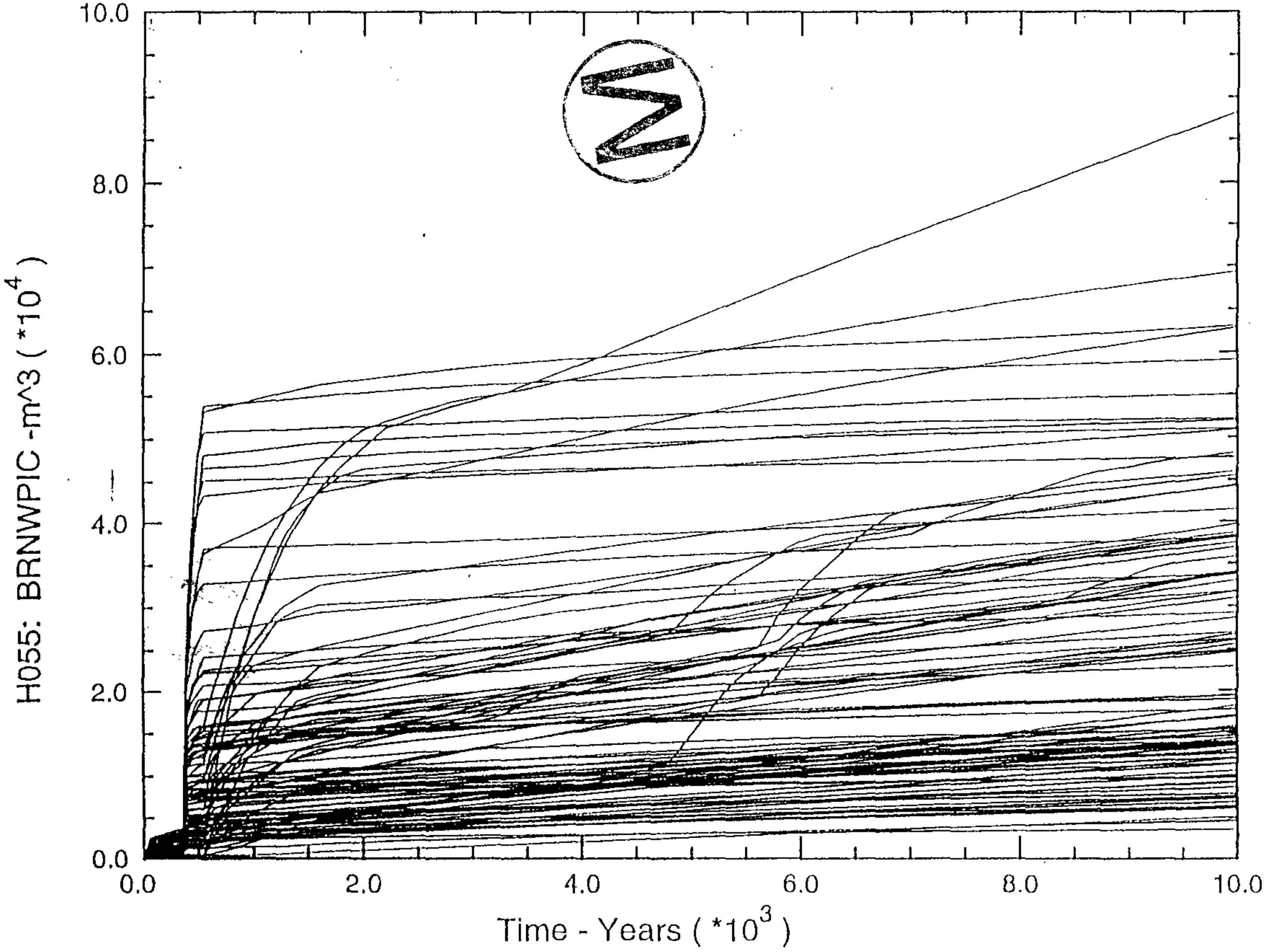
The maximum reaction rate and the inventory of $C_6H_{10}O_5$ in a single waste panel are estimated to be $1x10^5$ moles/year and $1.2x10^7$ moles (Wang & Brush, 1996; DOE/CAO, 1996). With $\Delta H = -3.1x10^5$ J/mole (Lide, 1994, p. 5-16 to 5-37), $\Delta T_{max}$, is estimated to be 0.8 K. Because of lack of thermodynamic data for cellulose materials, we here assume that the enthalpy of $C_6H_{10}O_5$ is approximately equal to that of $C_6H_{10}O_4$.

*(4) Aluminum corrosion:* $Al + 3H_2O \rightarrow Al(OH)_3 + 1.5\,H_2$

The inventory of Al in a single panel is about $8x10^6$ moles (DOE/CAO, 1996). Aluminum are present as foil in the waste and its thickness is estimated to be $2.54x10^{-4}$ cm. The total surface area of Al foil is thus estimated to be ~ $2.6x10^8$ $m^2$. With this high surface area and the measured corrosion rate (2.9 mole $H_2/m^2$/year, Telander & Westerman, 1996), Al corrosion reaction is expected to be limited by brine inflow, and the maximum corrosion rate is ~ $0.4x10^7$ moles/year. With $\Delta H = -\ 4.4x10^5$ J/mole (Drever, 1982, p. 351-356), $\Delta T_{max}$, is estimated to be 6 K.

gure 2. SNL WIPP PA96: BRAGFLO SIMULATIONS (CCA R1 S2)

Cumulative Brine Inflow into Waste Panel



The two brine-inflow-limited reactions - MgO hydration and Al corrosion - could possibly bring repository temperature up to 6 K. However, this temperature increase will not affect the overall repository performance, for two reasons: (1) The maximum temperature, if it is achieved, will be sustained only over a very short time period. For example, to achieve this temperature, Al has to be corroded completely within 2.5 years. After that, the accumulated heat will be dissipated away quickly. Thus, the maximum temperature, if it is attained, will last perhaps less than a year. (2) More importantly, because the two reactions are brine-limited, they will consume all free brine in the repository until all the reactants are completely consumed. Therefore, the maximum temperature will occur much earlier than enough free brine accumulates in the repository for the release of dissolved actinides. Based on the above calculations, the thermal effect of the other reactions, which are not limited by brine inflow and can last over a significant portion of 10000 year time period, are definitely negligible.

In conclusion, ignoring the thermal effect of chemical reactions (1 - 5) can not affect the overall repository performance assessment.

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