MASS-15.2.1 Current Studies of Sorption in the Culebra

Several factors affect the sorption of Pu, Am, U, Th, and Np, the elements for which K_d values are required in ~~performance assessment~~***PA*** for Culebra transport calculations (Ramsey 1996) including:

- the properties of the sorbents (solids) that will sorb actinides from solution,
- the composition of solutions that currently exist in the Culebra or could enter the Culebra after human intrusion into WIPP disposal rooms,
- the oxidation state of the sorbate (actinide elements) in the Culebra,
- dissolved actinide concentration,
- equilibration time, and
- direction of reaction (sorption versus desorption).

The two most important sorbents in the Culebra are dolomite, a carbonate mineral that constitutes most of the Culebra, and corrensite, an ordered mixture of chlorite and saponite associated with fracture surfaces and dispersed in the matrix (intact rock between the fractures) of the Culebra. Dolomite is important because it is by far the most abundant mineral in the Culebra. Corrensite is important because, although a minor constituent, it sorbs actinide elements more strongly than dolomite. The work of Sewards (1991) and Sewards et al. (1991, 1992) indicates that corrensite is associated with fracture surfaces and dispersed in the matrix at concentrations high enough to increase the retardation of Pu, Am, U, Th, and Np relative to that observed in laboratory studies with dolomite-rich rock. ***(Np was not transported in the 1996, the 2004 PA, or the 1997 PAVT, but K_ds were also determined for this element for completeness.)*** However, the DOE does not include K_ds for clay minerals in the ranges and probability distributions for the matrix K_ds ~~for~~ use***d*** in ~~performance assessment~~***PA*** calculations because laboratory data for clay-rich rock under expected Culebra conditions are insufficient at this time. Furthermore, the DOE does not take any credit for sorption by clay minerals associated with fracture surfaces. Omitting K_ds for clays is conservative.

The experimental basis for the ranges and probabilities of matrix distribution coefficients is documented in ***CCA MASS*** Attachment 15-1.

MASS-15.2.2 Historical Studies of Sorption in the Culebra

See CCA Appendix MASS, Section MASS.15.2.2 for historical information relating to the CCA Culebra conceptual model.

~~The DOE carried out several laboratory studies of sorption in the late 1970s and early 1980s (Serne et al. 1977; Paine and Dosch 1992; Dosch and Lynch 1978; Dosch 1979, 1980, 1981; Lynch and Dosch 1980; Lynch et al. 1981; Tien et al. 1983). These empirical studies used a variety of sorbents and solutions—including dolomitic, anhydritic, and clay-rich rocks and repository and Culebra brines—and in some cases included the effects of dissolved organics on~~

~~sorption. The DOE (1980) used some of these results for the 1980 WIPP Environmental Impact Statement (EIS). According to Lappin et al. (1989), the sorption model used by the DOE (1980) included a porous-medium approximation of the Culebra. Lappin et al. (1989) and the DOE Office of Environmental Restoration and Waste Management (1990) also used these results for the 1990 Supplemental EIS. For Pu, Am, U, Th, Np, and Cm, Lappin et al. (1989) and the DOE Office of Environmental Restoration and Waste Management (1990) included sorption by the matrix only, linear sorption isotherms, and instantaneous, reversible equilibrium in their model. For Ra and Pb, however, they assumed linear, instantaneous, reversible sorption by clay minerals in the matrix because there were no data available for sorption of these elements by dolomite.~~

~~The DOE and the state of New Mexico formally recognized deficiencies in the early sorption studies. In 1988, the DOE and the state of New Mexico modified the Consultation and Cooperation agreement to require New Mexico concurrence on any K_ds recommended for use in the final performance assessment. Papenguth and Behl (1996b) planned the current program (see below) in part to satisfy that agreement.~~

~~Soon after the agreement was reached, the DOE started a mechanistic sorption study, primarily at Stanford University (Lappin et al. 1989; Siegel et al. 1990; Park et al. 1992, 1995). The objective of this study is to develop a surface-complexation model for the sorption of UO_2^{2+} by corrensite, the dominant clay mineral in the Culebra. It is infeasible, however, to use this model in performance assessment calculations for three reasons:~~

- ~~laboratory data for clay-rich rock under expected Culebra conditions are insufficient at this time to include K_ds for clay minerals in performance assessment calculations;~~

- ~~the Stanford results pertain only to sorption of U(VI) and its oxidation-state analogs Pu(VI) and Np(VI), none of which will significantly affect the long-term performance of the WIPP; and~~

- ~~even if sorption of U(VI), Pu(VI), or Np(VI) did affect the long-term performance of the WIPP significantly, it would not be possible to incorporate a surface-complexation model in the Culebra flow and transport codes SECOFL2D and SECOTP2D.~~

~~At about the same time that the Stanford mechanistic sorption study began, the DOE convened an expert panel consisting of SNL staff to estimate ranges and probability distributions of K_ds for use in performance assessment. This panel estimated ranges and distributions of actinide K_ds for the Culebra as a whole and for the clay-rich fracture surfaces (Trauth et al. 1992). These values were used for the 1991 and 1992 calculations.~~

MASS-15.3 Colloidal Actinide Transport and Retardation in the Culebra

The purpose of this model is to represent the effects of colloidal actinide transport in the Culebra. This model is also discussed in Section 6.4.6.2.2 and Attachments 15-2, 15-8, and 15-9.

A particle is referred to as being in the colloidal state when the particle size lies roughly in the range between 1 ~~and 1,000~~ nanometers ***and 1 micron***. These particles are generally much larger than simple ions, and as a result, the transport behavior of colloids in groundwater systems can be quite different from that of dissolved species. In a groundwater system, colloids are essentially a third phase consisting of a mobile solid that can associate with or contain actinides and potentially increase transport rates slightly relative to the average groundwater velocity.

In the WIPP disposal system, for instance, colloids are often too large to pass through the small pore throats of diffusive porosity. Such colloids will be restricted to the advective portion of the flow system. Colloids may also be less reactive than dissolved actinides with the host rock. Therefore, even though a colloid is small enough to penetrate the diffusive porosity, the retardation coefficient associated with the colloid will in some cases be smaller than the retardation coefficient of the actinide associated with the colloid.

Colloid-facilitated actinide transport has not been included in ~~past performance assessment~~***the 1996 PA, the 2004 PA*** calculations***, or the 1997 PAVT*** because of a lack of adequate information to model this phenomenon and demonstrate its impact on compliance (see, for example, SNL, 1992-1993, Vol. 1, 4-12, line 29). Transport of actinides by colloidal particles has been recognized only relatively recently as a phenomenon of potential importance to the performance of nuclear waste repositories (Jacquier 1991; Avogadro and de Marsily 1984). In fact, the study of colloid-facilitated contaminant transport is a relatively new topic to the geosciences in general. Nyhan et al. (1985) was one of the first investigations to demonstrate the potential importance of colloid-facilitated radionuclide transport. Since then, a number of researchers have investigated colloids as a potential transport mechanism (for example, McCarthy and Zachara 1989; Corapcioglu and Jiang 1993; Grindrod 1993; Ibaraki and Sudicky 1995). Grindrod (1993) and Ibaraki and Sudicky (1995) addressed the topic of colloid-facilitated transport through fractured porous media. Consequently, their work is most applicable to the colloid-transport problem in the Culebra.

Among the most sophisticated and rigorous numerical models developed are those by van der Lee et al. (1993, 1994) and Bennett et al. (1993). Many of the colloid-transport numerical models described in the literature focus on simulating solute transport through fractured media with double-porosity flow characteristics, and they have been generalized to include unique features of colloid transport (for example, Hwang et al. 1989; Grindrod and Worth 1990; Light et al. 1990; Smith and Delgueldre 1993; Harmand and Sardin 1994). Some numerical models, such as the population-balance model by Travis and Nuttall (1985), assume equilibrium colloid concentrations. That is, the loss of colloidal particles by attachment to the medium wall is compensated by the generation of new colloidal particles by various mechanisms such as condensation and entrainment. The modeling approach developed by Travis and Nuttall (1985) is similar to the double-porosity transport model.

MASS-15.3.1 Experimental Results

As discussed in Section 6.4.6.2.2, the four types of colloids and colloidal sized particles modeled to be introduced to the Culebra are microbes, mineral fragments, humic substances, and actinide intrinsic colloids. To investigate the impact of these four colloid types on radionuclide transport in the Culebra, an experimental program was developed and implemented at SNL with significant contributions from Lawrence Livermore National Laboratory (LLNL), Battelle National Laboratory, Los Alamos National Laboratory (LANL), and Florida State University. The intent of this experimental program was to develop parameter ranges and distributions for the conceptual models discussed above. With the exception of the Pu (IV) polymer, the experimental results indicated that colloid-facilitated actinide transport is not a viable mechanism for actinide transport in the Culebra. Furthermore, the potential amount of Pu (IV) polymer that could be introduced to the Culebra was found to be insignificant with respect to the EPA normalized release limit. Consequently, colloid-facilitated actinide transport was not simulated in the ~~performance assessment~~***PA***.

The experimental results and implications ~~on performance assessment~~***for PA*** modeling are summarized as follows:

- Mineral fragments and microbes are attenuated so effectively it was deemed unnecessary to include them in the transport calculations (see ***CCA Appendix MASS,*** Attachments 15-8 and 15-9).

- The total potential amount of Pu (IV) polymer introduced to the Culebra was found to be insignificant with respect to the EPA normalized release limit (Attachment 15-8). Therefore, the contribution of Pu (IV) polymer to the integrated discharge was disregarded in the ~~performance assessment~~***PA***.

- Under neutral to slightly basic brine conditions, the presence of humic substances in the brine did not influence the sorption behavior of dissolved actinides. Results indicate that at these geochemical conditions, humic substances were not effective complexants in the presence of dolomite (Attachment 15-8). Therefore, actinides associated with humic substances are assumed to disassociate upon entering the Culebra.

MASS-15.3.2 Indigenous Colloidal Transport

In an intrusion scenario at the WIPP, as dissolved actinide elements are introduced to the Culebra, it is possible that those dissolved actinides could sorb onto a separate population of indigenous mineral fragments, microbes, and humic substances. The physical and chemical behavior of these newly formed actinide-bearing colloidal particles will be nearly identical to the behavior of colloids introduced from the repository. Microbes and mineral fragments will be rapidly filtered out of the advective flow domain; hence, disregarding the interaction between dissolved actinides and these types of colloids is considered to be a conservative approach. Experimental results indicate that humic substances do not interact with dissolved actinides under the expected Culebra geochemical conditions. Consequently, the quantity of newly formed actinide-bearing humics will be insignificant.

MASS-15.3.3 Alternative Approaches Considered

As discussed above, results of experimental studies show that colloidal actinides are strongly attenuated or present in negligible concentrations, making it unnecessary to include them in ~~performance assessment~~***PA*** simulations. The following section describes the three alternative transport conceptual models considered prior to the completion of these experimental results.

After the introduction of colloidal actinides and dissolved actinides into the Culebra, realistically a new equilibrium condition will be established, with the stipulation that the total concentration of actinide must be preserved. As in the repository, quantifying an equilibrium assemblage is not practicable.

Three approaches were considered to quantify colloid-facilitated actinide transport at the WIPP. First, the transport of one or more types of actinide-bearing colloidal particles in the Culebra could be assumed to be instantaneous. In other words, as actinides associated with that type of colloidal particle migrate to the Culebra from the repository, or are generated within the Culebra, the mass of actinides associated with those colloidal particles becomes part of the integrated release of actinides at the accessible environment boundary. This approach can be useful if the concentrations of actinides associated with one or more types of colloidal particles are very low. Treating colloid-facilitated actinide transport as instantaneous, however, is a significant shortcoming, because of the potentially large expected retardation effects of colloidal particles.

Second, SECOTP2D and supporting codes could be used to simulate the effects of one or more of the colloid retardation phenomena (Ramsey 1996). The double-porosity advection and diffusion equation solved by SECOTP2D can simulate colloid sorption in the matrix and to the fracture walls. The code can also model colloid filtration using the decay term of the governing equation. For colloids considered too large to diffuse into the matrix, matrix diffusion can be disabled by setting the matrix tortuosity to zero. This approach was used for some calculations completed in 1994. Specifically, microbes, because of their relatively large size, were excluded from matrix diffusion and limited to advective flow in fractures. Humic substances were allowed to diffuse into intercrystalline pores, but at a reduced rate relative to dissolved actinide species.

This approach requires a number of simplifying assumptions under the presumption they are conservative with respect to the integrated release of radionuclides. The first assumption is that the dissolved concentration will be greatest at the source point and therefore, the concentration of radionuclides associated with colloids will be greatest at the source as well. Second, a radionuclide associated with a colloid is assumed to remain fixed to that colloid throughout the simulation. Given these assumptions, the colloidal actinide concentration is no longer a function of the dissolved actinide concentration, and it is not necessary to solve the dissolved species transport problem and the colloid transport problem simultaneously. As a result, the standard advection-diffusion transport equation can be used to predict colloid transport and compute integrated colloid releases. Given the initial concentration of radionuclides sorbed to each specific type of colloid, the integrated colloid release can be converted to an integrated radionuclide release by postprocessing the colloid transport results. Radionuclide decay can also be accounted for in postprocessing.

The third assumption is that colloid-facilitated actinide transport could be quantified by a rigorous numerical modeling code developed for the WIPP. Such a rigorous transport model would address all physical and chemical processes that could affect the movement and fate of the four colloidal particle types, including colloid generation; interactions with solutes, the dispersant, and rock; advection; dispersion; diffusion; filtration; gravitational settling; attachment and detachment; adsorption and desorption; coagulation; flocculation; and peptization. Ideally, permeability reduction caused by pore clogging by colloids, which would affect solute transport as well, would also be considered. Currently available models do not include all of these processes (see ***CCA Appendix MASS,*** Attachments 15-2, 15-8, and 15-9).

The most practical approach to evaluating the transport of colloidal actinides is the second option presented above, using the SECOTP2D code. Where possible, the DOE considered reducing the number of phenomena treated in the transport code and address them in the source term. For example, the effect of ionic strength on colloid stability would have been included in the colloid source term. Retardation of colloidal particles was to be quantified using a retardation factor, and filtration was to be quantified through the decay term.

MASS-15.4 Subsidence Caused by Potash Mining in the Culebra

This model incorporates the effects of potash mining in the McNutt on disposal system performance (see Appendix ***PA, Attachment*** SCR, ***FEPs H13, H37, and H38***~~Sections SCR.3.2.2 and SCR.3.3.2~~). 40 CFR Part 194 provides a conceptual model and parts of a mathematical model for these effects. The DOE has implemented the EPA conceptual model to be consistent with EPA criteria and guidance. It is described in Section 6.4.6.2.3 of this ***recertification*** application. Additional information on the implementation of the mining subsidence model is available in ***Appendix PA, Attachment TFIELD, Section TFIELD-9.0; CCA Appendix MASS,*** Attachments 15-4 and 15-*7;* and ***Wallace (1996)*** ~~Bertram (1995)~~.

The principal parameter in this model is the range assigned to a factor by which hydraulic conductivity in the Culebra is increased (***CCA Appendix MASS,*** Attachment 15-4). As allowed in supplementary information to 40 CFR Part 194, it is the only parameter changed to account for the effects of mining.

Mining in the McNutt has been considered in the performance of the WIPP since the original siting activities. Siting criteria for both the site abandoned in 1975 and the current site included setbacks from active mines. (See, for example, Section MASS~~.~~-2*.0*.) The 1980 FEIS for the WIPP (DOE 1980) considered the possibility of an indirect dose arising from the effects of solution mining for potash or halite; it concluded that direct access of waste by solution mining for potash was not likely because of the methods that would be used to control the flow of solvent through the formation. ~~The DOE is not aware of solution mining for potash or other minerals in the Salado within the Delaware Basin at this time.~~ ***See Appendix PA, Attachment SCR (FEPs H58 and H59).***

Mining has been included in scenario development for the WIPP since the earliest work on this topic (for example, Hunter 1989; Marietta et al. 1989; Guzowski 1990; Tierney 1991; and WIPP Performance Assessment Division 1991). These early scenario developments considered both solution and room-and-pillar mining. The focus was generally on effects of mining outside the disposal system. The two primary effects of mining considered were changes in the hydraulic conductivity of the Culebra or other units and changes in recharge as a result of surface subsidence. These mining effects were not formally incorporated into quantitative assessment of repository performance in preliminary ~~performance assessments~~***PAs***.

The inclusion of mining in ~~performance assessment~~***PA*** satisfies the criteria of 40 CFR Part 194 to consider the effects of this activity on the disposal system.

MASS-16*.0* INTRUSION BOREHOLE

The inclusion of intrusion boreholes in ~~performance assessment~~***PA*** adds to the number of release pathways for radionuclides from the disposal system. Direct releases to the surface may occur during drilling as particulate material from cuttings, cavings, and spall are carried to the surface. Also, dissolved actinides may be carried to the surface in brine during drilling. Once abandoned, the borehole presents a possible long-term pathway for fluid flow, such as might occur between a hypothetical Castile brine reservoir, the repository, and overlying units. This topic is also addressed in Chapter 6.0, (Section 6.4.7) and Appendix ***PA Attachment*** SCR (***FEPs H1 and H21***~~Sections SCR.3.2.1 and SCR.3.3.1~~).

MASS-16.1 Cuttings, Cavings, and Spall Releases during Drilling

These models estimate the quantity of actinides released as solids directly to the surface during drilling through the repository by three mechanisms: the drillbit boring through the waste (cuttings), the drilling fluid eroding the walls of the borehole (cavings), and high repository gas pressure causing solid material failure and entrainment into the drilling fluid in the wellbore (spallings). See Section 6.4.7.1 and references to other appendices cited in that section for additional information. Stochastic uncertainty with respect to parameters relevant to these release mechanisms is addressed in Section 6.4.12. The conceptual model for cuttings, cavings, and spallings is discussed in three parts because of the differing process by which the three types of material are produced.

Cuttings are materials removed to the surface through drilling mud by the direct mechanical action of the drill bit. The volume of waste removed to the surface is a function of the repository height and the drill bit area. The cuttings model has as a principal parameter the diameter of the drill bit (see Appendix DATA, Attachment A).

Cavings are materials introduced into the drilling mud by the erosive action of circulating drilling fluid on the waste in the walls of the borehole annulus. Erosion is driven solely by the shearing action of the drilling fluid (or mud) as it moves up the borehole annulus. Shearing may be caused by either laminar or turbulent flow. Repository-pressure effects on cavings, which are negligible, are covered by the spall process. The principal parameters in the cavings model are the properties of the drilling mud, drilling rates, the drill string angular velocity, and the shear resistance of the waste. See Appendix PA, Attachment PAR (Tables PAR-13 and PAR-18) for details on the sampled parameters used in the cavings model, the drill string angular velocity, and the effective shear resistance to erosion.

Spallings are solids introduced into the wellbore by the fluid pressure difference between the repository and the bottom of the wellbore. If the repository pressure is sufficiently high (~ >12 MPa) relative to the well bottom hole pressure (~8 MPa), the stress state in the repository may cause repository solids to fail in the vicinity of the wellbore. In turn, these solids may become entrained in the gas flowing toward the well, ultimately to be carried up to the land surface, constituting a release. The principal parameters in the spallings model are the gas pressure in the repository when it is penetrated and properties of the waste such as permeability, tensile strength, and particle diameter. Because the release associated with spalling is sensitive to gas pressure in the repository, it is strongly coupled to the BRAGFLO-calculated conditions in the repository at the time of penetration.

MASS-16.1.1 Historical Context of Cuttings, Cavings and Spallings Models

Cuttings and cavings releases are straightforward. The analytical equations governing erosion (cavings) based on laminar and turbulent flow (Appendix PA, Section PA-4.5) have been implemented in the code CUTTINGS_S. Using selected input based on assumed physical properties of the waste and other drilling parameters, this code calculates the final caved diameter of the borehole that intersects the waste.

The various approaches used for spallings up to the CCA PA are documented in CCA Appendix MASS.16.1.1. Since the CCA PA, the spallings model has been extensively revised and has changed fundamentally from an end-state erosional model to a mechanically based coupled material failure and transport model (WIPP PA 2003a). This model is implemented in a new code, DRSPALL. The following discussion traces the historical steps from the CCA erosional model to DRSPALL.

According to the WIPP Conceptual Models Peer Review Report (CCA Section 9.3.1.2.7), the three primary objections to the erosional spallings model were; (1) channel flow scenario needed additional validation, (2) waste erosion resistance process and parameters had not been adequately evaluated, and (3) assumptions concerning waste degradation and strength. Though the strength value used, 1 lb/in^2, was consistent with the strength of soils, salt and clay mixtures, and similar mixtures with MgO (see CCA Appendix PEER, Section 2.6 for Berglund 1996), the peer review panel was not convinced of the applicability of this value in the model (Wilson et al. 1996b). Hansen et al. (1997) decided to revise the approach to estimating spall release and embarked on a two-part effort that sought to (1) derive mechanical strength estimates from laboratory measurements on surrogate WIPP wastes, and (2) develop a new mechanically-based model for spall that attempts to encompass the entire system response from bit penetration to near steady state rather than just the end state, as done in the erosional model. The results of the model development efforts were implemented in the code GASOUT (Hansen et al. 1997, Appendix C).

MASS-16.1.2 Waste Mechanistic Properties

The spalling event can occur only in cases that combine high pressure with highly degraded waste. A systematic approach was implemented to characterize the waste after compaction, corrosion, and microbial consumption through the used of waste surrogate materials. The primary emphasis of the waste surrogate testing was devoted to quantifying tensile strength, although many other characteristics, such as particle size, permeability, and heterogeneity, will greatly influence potential spall release. Utilizing a projected inventory of waste materials placed in the repository and assuming extensive degradation, recipes (mixtures) for surrogate products were determined. Surrogate recipes derived from corrosion of 50 percent and 100 percent of the Fe-based inventory were fabricated and mechanically tested using standard laboratory procedures (Hansen et al. 1997).

Degraded waste strength was recognized as a key parameter in a WIPP spallings model (Wilson et al. 1996a, 1996b). Lacking, however, were compelling data to validate the value of tensile strength T_o = 1 lb/in^2 used in the CCA erosional model. In an attempt to build an understanding of the mechanical properties of degraded WIPP wastes, Hansen et al. (1997)

developed a test methodology to construct and examine surrogate wastes. They scanned the inventory of WIPP wastes and prepared recipes for various surrogate wastes. A wide variety of materials were cut, shred, compressed, and aged in the laboratory to create specimens appropriate for standard laboratory measurements such as tensile and compression tests. Overall, results from 38 specimens were reported in Hansen et al. (1997) quantifying properties including tensile strength, cohesion, friction angle, Poisson's ratio, and Biot's constant. These data helped to make the case that the $T_o = 1$ lb/in^2 value used in the CCA was indeed conservative.

Subsurface processes leading to extensive degradation are based on several contributing conditions including ample brine availability, extensive microbial activity, corrosion, and the absence of cementation and salt encapsulation effects. Property values from these surrogate materials are selected to represent the worst-case response to the process being investigated (Hansen et al. 2003b). In terms of the degraded waste properties, the model is highly conservative.

MASS-16.1.3 New Mechanistic Model for Spall

In addition to the work on waste degradation, Hansen's team also laid the groundwork for a new approach to modeling the WIPP spallings process. Instead of focusing on the end state after penetration, as is done in the erosional model, the new effort sought to capture the system behavior from just before penetration through to the end state. In doing so, many more phenomena were included in the model. Considered in this new conceptual model was unsteady, convergent gas flow from the repository toward the wellbore that caused mechanical stress and potential failure of solids near the face of the wellbore. Pressure in the cavity at the point of penetration was balanced by the mud column in the wellbore and the repository pressure. This represented a more complex modeling approach, and was developed sufficiently to satisfy the peer review panel that convened in April, 1997 that the spallings release values used in the CCA were conservative (Wilson et al. 1997).

The new spall model, DRSPALL (WIPP PA 2003a) is based on a predecessor code called GASOUT (Hansen et al. 1997, Appendix C). DRSPALL builds upon GASOUT by:

1. *Adding a wellbore flow model that transports mud, repository gas, and waste solids from repository level to the land surface; and*

2. *Adding a fluidized bed model that evaluates the potential for failed particulate waste to fluidize and become entrained in the wellbore flow.*

The wellbore flow model in DRSPALL utilizes one-dimensional geometry with a compressible, viscous, isothermal, homogeneous mixture of mud, gas, and solids. Standard mass and momentum balance, friction loss, and slurry viscosity equations are used. Wellbore flow model results were successfully verified against those from an independent commercial code for several test problems (WIPP PA 2003b).

DRSPALL applies the fluidized bed theory to determine the mobilization of failed material to the flow stream in the wellbore. If the escaping gas velocity exceeds the minimum fluidization velocity, failed material is fluidized and entrained for transport at the land surface. If gas

velocity is too low to fluidize the bedded material, however, the cavity size is allowed to stabilize The spall volumes predicted by DRSPALL are based on conservative assumptions for material properties and for the flow geometry within the repository.

- ***The particle size distribution for spallings is based on a detailed analysis (Wang 1997) of data from an expert elicitation (DOE 1997). This analysis considered several limiting cases in developing a conservative distribution for mean particle size ranging from 1 mm to 10 cm (Hansen et al. 2003b).***

- ***The shape factor for fluidization of particles has a potential range from 0 to 1.0. Smaller values of the shape factor denote particles that are less spherical, and therefore more easily fluidized and transported in the flow. The shape factor is conservatively set to a value of 0.1 for CRA-2004 (Lord 2003).***

- ***The tensile strength of the waste assigned for the spalling process is uncertain, ranging from 0.12 MPa to 0.17 MPa (Hansen et al. 2003b). Tensile strength data was measured in laboratory experiments on surrogate materials that were chosen to conservatively represent highly degraded residuals from typical wastes. The given range is felt to represent extreme, low-end tensile strengths because it does not account for several strengthening mechanisms, such as MgO hydration and halite precipitation/cementation (Hansen et al. 1997).***

- ***DRSPALL uses a hemispherical geometry (one-dimensional spherical symmetry) for the flow field and cavity in the waste. This conceptual model is appropriate when the drill bit first penetrates the repository. But as the drill bit passes completely through the compacted waste, the flow field will transition toward a cylindrically symmetric geometry. This transition is important because the largest spall release volumes are predicted to occur at late times, well after the drillbit has penetrated through the waste, and because the spall volumes predicted for a cylindrical geometry are less than for the hemispherical geometry (Lord et al. 2003).***

In spite of this transition, the hemispherical geometry is used for the CRA-2004 spallings release calculations because it produces conservative results. Fifty calculations performed with DRSPALL in both the hemispherical and cylindrical flow geometries demonstrated that the spall volumes predicted with the hemispherical geometry are always larger than those for the cylindrical geometry (Lord and Rudeen 2003, Section 3.3 Sensitivity Analysis Report Part 2). In fact, the spall volumes are zero for all 50 realizations with a cylindrical geometry, which indicates that the likelihood of spalling is quite small in this geometry. It follows that the hemispherical geometry results in spall volumes that are conservative relative to the cylindrical geometry.

There is no consensus about how the driller will act as the drill approaches the waste horizon; that is, whether he or she will be able anticipate the presence of the gas-filled repository, or if he or she can or will control the drilling process once penetration occurs. For the WIPP intrusion scenarios, the conceptual model assumes the worst possible limiting situation, in which the borehole is driven through the waste by a driller without any knowledge of the

existence of the repository, and the driller is unable or unwilling to control the subsequent gas release.

In summary, the conservative assumptions for waste properties, the waste flow geometry and the driller's actions provide very conservative spalling release volumes for CRA-2004 (see also Appendix PA, Section PA-4.6 for a description of the spallings model and Section 9.3.1.3.5.5 for the results of the new spallings model peer review).

MASS-16.1.4 Calculation of Cuttings, Cavings, and Spall Releases

As detailed in Appendix PA, Section PA-6.7, cuttings and cavings releases for intrusions into contact handled (CH)-TRU waste are computed by multiplying the volume released (calculated by the code CUTTINGS_S) with the radioactivity in three independently-selected waste streams, consistent with the conceptual assumption that waste is randomly placed within the repository. The effect of this assumption on PA results was examined in a separate PA (Hansen et al. 2003a) in which cuttings and cavings releases were computed by assuming that each intrusion encounters only a single waste stream. The differences in repository performance (determined by comparing the mean CCDFs for releases) were determined to be minor. For more details on the analysis, see Section MASS-21.0.

Because spallings may releases a relatively large volume of material (exceeding 4 m^3), spallings releases for intrusions into CH-TRU waste are computed by multiplying the volume of spalled material with the average concentration of radioactivity in the waste at the time of the intrusion. A separate PA (Hansen et al. 2003a) compared spallings releases computed using the average concentration of radioactivity in the waste to spallings releases computed by using the radioactivity of a single, randomly selected single waste stream. The analysis determined that the assumption had only a minor effect on the mean CCDF for releases. For more details on the analysis, see Section MASS-21.0.

~~The purpose of these models is to estimate the quantity of actinides released directly to the surface during drilling through the repository by three mechanisms: the drillbit boring through the waste (cuttings), the drilling fluid eroding the walls of the borehole (cavings), and gas movement forcing particulate matter into the circulating drilling fluid (spallings). See Section 6.4.7.1 and references to other appendices cited in that section for additional information. Stochastic uncertainty with respect to parameters relevant to these release mechanisms is addressed in Section 6.4.12.~~

~~The conceptual model for cuttings, cavings, and spallings is discussed in three parts because of the differing process by which the three types of material are produced.~~

~~Cuttings are materials removed to the surface through drilling mud by the direct mechanical action of the drill bit. The volume of waste removed to the surface is a function of the compacted repository height, the porosity of waste at the time of intrusion, and the drill bit area. The radioactivity of waste removed to the surface is probabilistically determined based on the distribution of waste radioactivity expected in the WIPP.~~

~~Cavings are materials introduced into the drilling mud by the erosive action of circulating drilling fluid on the waste in the walls of the borehole annulus. Erosion is driven solely by the~~

shearing action of the drilling fluid (or mud) as it moves up the borehole annulus. Shearing may be caused by either laminar or turbulent flow. Repository pressure effects on cavings, which are negligible, are covered by the spall process.

Spallings are the particulate material introduced into drilling mud by the movement of gas from the waste into the borehole annulus. After the drill bit enters the repository, pressure gradients generated by the flow of gas toward the borehole fracture the waste material, permitting the escaping gas to flow within fractures rather than through a porous matrix. Consequently, the intrinsic permeability of the matrix does not restrict gas flow, and the gas pressure at the borehole entrance to the repository can be assumed to be the initial gas pressure in the repository. The gas flow velocity up the borehole is governed by the isothermal flow of gas in a long tube of a given cross-sectional area, tube roughness, and gas pressure at the borehole entrance. The mass-flow rate of gas in the fractured waste at any radial cross-section is equal to the mass-flow rate up the borehole. Radial gas flow within the fractures in the waste matrix erode and widen the fractures. Erosion is assumed to occur if the fracture gas velocity exceeds a threshold velocity related to the terminal velocity of a waste particle at the fracture surface and to the cohesive strength afforded by moisture in the matrix.

The cuttings model has as a principal parameter the diameter of the drill bit, which according to current practice is constant. This model interacts with the conditions in the repository as calculated by BRAGFLO because the porosity and height of the repository are necessary to calculate the volume of waste removed.

The principal parameters in the cavings model are the properties of the drilling mud, drilling rates, and the shear resistance of the waste. See Appendix PAR (Parameter 33) for details on the sampled parameter used in the cavings model, effective shear resistance to erosion.

The principal parameters in the spallings model are the gas pressure in the repository when it is penetrated and properties of the waste such as particle diameters and erosive properties. Appendix PAR (Parameter 32) provides information on the waste particle diameter, which is a sampled parameter in the spallings model. Because the release associated with spalling is sensitive to gas pressure in the repository, it is strongly coupled to the BRAGFLO-calculated conditions in the repository at the time of penetration. In particular, the spall release may be sensitive to whether the repository has been penetrated previously by another borehole.

Several factors contribute to model uncertainty, principally the undefined nature and complexity of the waste, both in its initial state and during its alteration by chemical and biological processes. Even the most basic information is lacking, such as chemical form, grain size (if the material is granular), partially biodegraded decomposed form, density, cohesion, etc. In the absence of such information, property values typical of surrogate materials are selected to represent the worst case response to the process being investigated (see Appendix PAR, Table PAR-11; Chapter 9.0, Section 9.3.4.4; and Appendix WCA, Section WCA.5.2). In this sense, the model is highly conservative.

Another uncertainty arises from the drilling scenario assumptions for application of the model. There is no consensus about how the driller will act as the drill approaches the waste horizon, that is, whether he will be able anticipate the presence of the gas-filled repository, much less control the drilling process once penetration occurs. In consequence, the conceptual model assumes the worst possible limiting situation, in which the borehole is driven almost instantaneously through the waste by a driller without any knowledge of the existence of the repository, and the driller is unable to control the subsequent gas release.

The scale-up from a model qualified on laboratory samples to the full-scale configuration of a drill penetrating the waste gives rise to another uncertainty, the possibility of improper scaling. However, the adverse effect of improper scaling on the amount of waste released is considered to be negligible because of the conservatism of the material and drilling scenario assumptions.

MASS.16.1.1 Historical Context of Cuttings, Cavings, and Spallings Models

Releases of cuttings and cavings are straightforward and have been considered in performance analyses since the beginning of direct release evaluation. The analytical equations governing erosion (cavings) based on laminar and turbulent flow (Berglund 1992, Section 2.2) have been implemented in the code CUTTINGS_S. Using appropriately selected input based on assumed physical properties of the waste and other drilling parameters, this code calculates the final caved diameter of the borehole that passes through the waste. Although certain features of the analysis, such as whether the flow of the drilling fluid should be modeled as laminar or turbulent and what drilling parameters might be valid near the WIPP repository, have been debated, the basic model has been generally accepted. The amount of material predicted to be released by cavings is small, and therefore this contribution to surface release has never been considered to be critical.

The conceptual model of the release of waste by spalling has been changed several times during its development. Early spall conceptual model development focused on transient unrestrained outgasing leading to the spall (dynamic fracture) of porous cohesive granular media (Berglund 1992, Section 3.3). An experimental program related to model development focused on almost instantaneous depressurization and was limited to a one-dimensional linear sample configuration. The pore pressures required to cause spall or dynamic fracture could be closely approximated using the tensile strength of the porous soil medium (Berglund and Lenke 1995), but the model was complex and could not be directly related to an intrusion event. In addition, although the experimental observations showed fracturing under instantaneous release of gas pressure, sample-preparation factors were largely responsible for the locations of the fractures. The fracture patterns also depended on the one-dimensional nature of the experiments, and the model did not explain how the fractured material was removed.

Subsequently, the dynamic fracture spall model was replaced with a more general three-part model based on the premise that the waste could be removed by any one of three mechanisms: blowout, stuck pipe, and gas-flow assisted erosion (as the result of gas-induced spall). Which mechanism will dominate depends on the permeability and pressure drop at the borehole. Well blowout, an uncontrolled gas release from the well, was considered the dominant mechanism. The two remaining mechanisms, stuck pipe and gas-flow assisted erosion, were not thought to be important because they would occur at waste permeabilities of less than 10^{-16} square meters, much lower than is expected for the waste (1.7×10^{-13} square meters). Consequently, conceptual-model development has focused on the blowout mechanism for removing waste.

Once the DOE concluded that blowout was the principal cause of direct release of waste by spalling, the nature of the gas flow and the entrainment properties of the waste became the focus of subsequent model development. The first model, used in analyses in 1994, was simplistic. Release was defined in this model by how much gas flowed out into the borehole and an assumed amount of solids entrained in it over a prescribed time period. The time limit for release assumed in the calculations was 5 minutes, the time estimated for the driller to close the blowout preventers and start weighting up the drilling mud. Entrainment was a sampled percentage ranging from 0 to 10 percent. Defending the time limit for release was particularly difficult because opinions about how long it would take before the driller controlled the well varied widely. In addition, the model was not self-limiting, in the sense that release would continue for as long as the unchecked gas flow was assumed to continue, and quantification of the entrainment percentage was of concern.

To respond to these concerns, model development for release continued. A more-detailed model was developed based on the observation that a critical entrainment or lofting (terminal) velocity represents a threshold erosion condition. This value of the gas velocity defines whether solid particulate matter is separated from the bulk waste. Once separated, the material is assumed to be entrained in the gas and carried up the borehole to the ground surface (Berglund and Lenke 1995, Section 6.1, 33 – 39). Because gas velocities below this threshold can remove no solids, the removal process is self-limiting: gas velocity decreases as a function of distance from the borehole, eventually dropping below the entrainment velocity threshold and terminating the process.

The first version of the steady-state model incorporating the terminal velocity release process assumed that gas would flow uniformly through the waste and out the borehole. It was based on the fact that the velocity of the gas decreases with distance from the borehole, because of the symmetry of the gas flow field. The flow velocity is greatest at the borehole boundary and decreases with distance away from it. Therefore, at some point sufficiently remote from the borehole, the gas velocity just equals the critical entrainment (terminal) velocity. All material closer to the borehole was assumed to be eroded and lofted up the borehole, but the gas velocity in all material farther from the borehole was too low to cause erosion. This hypothesis permitted a calculation of how much material would be released in connection with an assumed gas-pressure drop in the waste disposal region.

An experimental program was designed to confirm the model using a test apparatus to simulate gas flow through the waste and up the borehole (Lenke and Berglund 1995). The model-confirmation process was to first experimentally determine the entrainment velocity characteristics of the material, and then apply these data to the model to predict the amount of release expected for various boundary pressures. Boundary pressures were then experimentally applied to the samples in the experimental blowout device, and the amounts of eroded material were determined assuming uniform Darcy flow. The confirmation criterion was that if the measured amount of lofted material was less than the predicted amount of erosion then the model was considered confirmed. Confirmation was never possible, however, because the material release tests revealed that the assumption of uniform gas flow through the waste was not reflected by the response of the material. Instead of formation and expansion of a cavity left behind by eroded material, post-test observations showed that the gas instead created flow channels that increased in thickness as erosion proceeded. Releases were greater than expected

~~because gas velocity in the channels was greater than it would have been had gas flowed through the bulk of the material (Lenke and Berglund 1995, 14). Channel flow was consistent with the heterogeneity of the waste.~~

~~The experimental observation of flow-channels formation by erosion forced another iteration in blowout-model development to make the model consistent with material response. The new model is used in performance assessment and is documented in Appendix CUTTINGS (Section 4).~~

~~Including a channel-flow mechanism in the model requires either precise definition of the number, geometric configuration, and location of all the channels before they form, which is not technically feasible, or scaling the model results in some manner to reflect the channeling process. The scaling method was adopted, adjusting the predicted releases to agree with experimental release observations. Although the uniform-flow model was independent of experiments, in the sense that release predictions did not require direct data from the tests, a coupling between experimental results and the model was necessary for scaling. This was accomplished by introducing certain experimentally determined scaling constants into the model (see Appendix CUTTINGS). The model is applied to different gases and solid materials by prescribing well-defined material properties, such as particle size and density, viscosity, and cementation tensile strength. The scaling factors are the only parameters of the model not directly related to geometry or material properties, but they are necessary to represent the way channels for gas flow are likely to develop.~~

MASS-16.2 Direct Brine Releases during Drilling

This model provides a series of calculations to estimate the quantity of brine released directly to the surface during drilling. Direct brine releases ***(DBRs)*** may occur when a driller penetrates the WIPP and unknowingly brings contaminated brine to the surface during drilling~~.~~ (~~T~~***t***hese releases are not accounted for in the cuttings, cavings and spallings calculations, which model only the solids removed during drilling~~.~~)***. Appendix PA, Section PA-4.7 described the DBR model used for the 2004 PA. CCA Appendix MASS,*** Attachment 16-2 describes the direct brine release model used for ***the 1996 PA*** ~~this performance assessment~~. The conceptual model ***for DBRs*** is ~~also~~ discussed in Section 6.4.7.1.1.

Uncertainty in the BRAGFLO direct-brine-release calculations is captured in the 10,000-year BRAGFLO calculations from which the initial and boundary conditions are derived. The model parameters that have the most influence on the direct brine releases are repository pressure and brine saturation at time of intrusion. Brine saturation is influenced by many factors, including Salado and marker bed permeability and gas-generation rates (for undisturbed calculations). For E1 and E2 intrusions, Castile brine-reservoir pressure and volume and abandoned borehole permeabilities influence conditions for the second and subsequent intrusions. Dip in the repository (hence the location of intrusions), two-phase flow parameters (residual brine and gas saturation), time of intrusion, and duration of flow have lesser impacts on brine releases.

To account for changes in the BRAGFLO model (see Section MASS-2.0), the implementation of the DBR model has been adjusted for the CRA 2004-PA. Figure MASS-9 shows the DBR

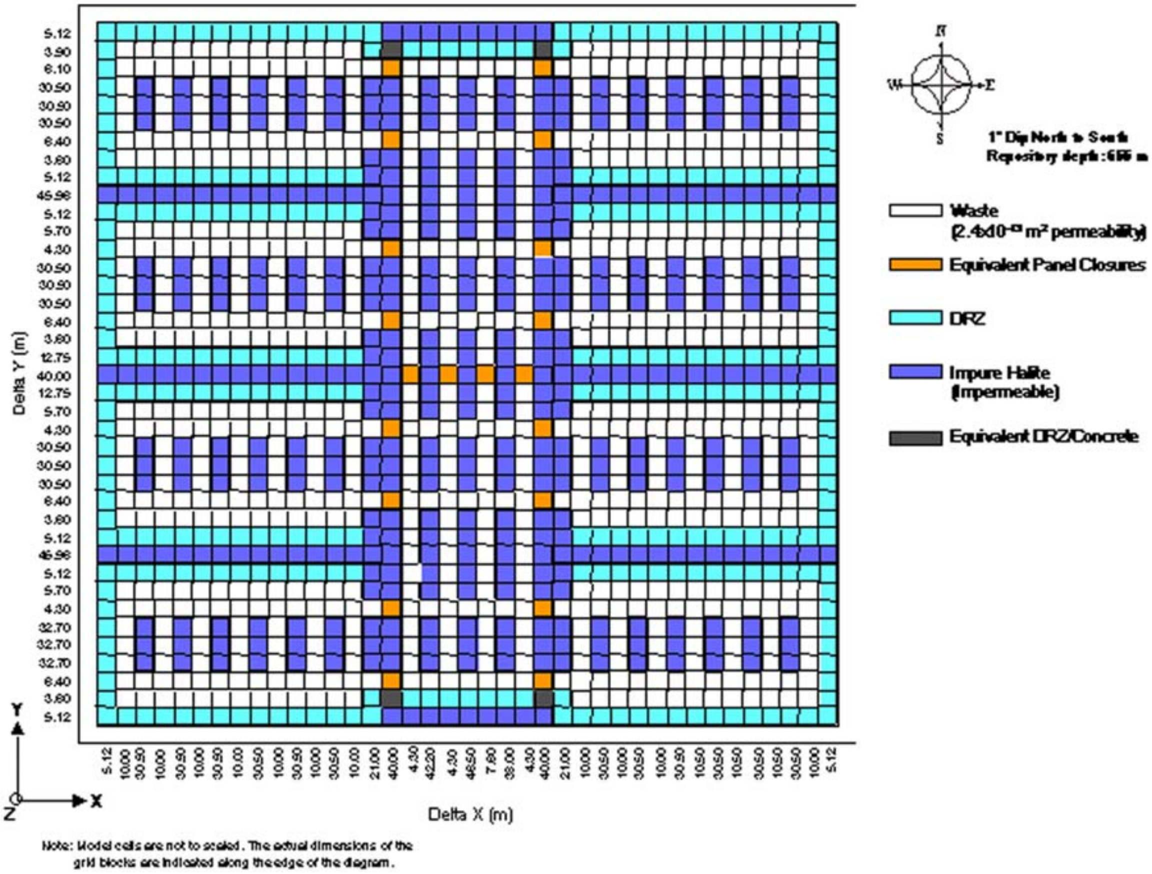

Figure MASS-9. Repository-Scale Horizontal BRAGFLO Mesh Used for Direct Brine Release Calculations

grid used in the 2004 PA. The grid dimensions and resolution are the same as in the CCA PA, but the material parameters assigned to the panel closures have been changed to be more consistent with the conceptual model for the Option D panel closures. In addition, the material parameters assigned to the DRZ have been changed to more consistently represent the DRZ. In the CCA PA, the pillars between rooms and the halite separating panels were assigned properties consistent with the DRZ material in the BRAGFLO grid. The DRZ permeability used in the CCA (10^{-15} m^2) was low enough that brine did not flow between panels during the 11-day DBR calculations. When the permeability of the DRZ was changed in the PAVT (from a constant value of 10^{-15} m^2 to a sampled value between $10^{-19.4}$ m^2 and $10^{-12.5}$ m^2), realizations with high DRZ permeability allowed brine flow between panels during the 11-day period for DBR calculations. It is not reasonable to model the halite between panels as DRZ, since the DRZ would extend only a few meters into the 60-m thick ribs. Consequently, the material parameters assigned to cells separating panels were changed to be representative of undisturbed halite, rather than DRZ. Stein (2003b) provides details on the material parameters used in the DBR calculation and the rationale for the parameter values.

~~MASS.16.2.1 Historical Context of the Direct Brine Release Model~~

~~The direct brine release model is a relatively new development in WIPP performance assessments, and this performance assessment is the first one to incorporate this mechanism of release. Prior to using the current model in this performance assessment, several iterations of models were performed. At first, a simplistic cylindrical (radial) BRAGFLO model was used to represent the excavated volume of one intruded panel, but this was inadequate to capture the effects of heterogeneities within the site. This model was replaced with the current repository scale mesh representing the configuration of the WIPP excavation, accounting for drifts, passageways, closures, pillars and rooms, and formation dip in the waste region. The current mesh reflects the configuration used by the DOE in this application, with flow unaffected by backfill within the panels. In addition, the vertical wellbore flow model is coupled to the BRAGFLO mesh, and the effects of solids removal caused by cavings and spall are examined (CUTTINGS_S code). Boundary conditions can account for two intrusions in a single panel, one of which connects to a brine reservoir.~~

~~The assumptions used in the models are based on current drilling practices in the Delaware Basin (see Appendix DEL). The wellbore model description assumes a typical WIPP-area oil or gas well completion, including bit size, casing size and depths, drilling mud, etc. The duration of flow is based on how a present-day driller might react to the pressures and flows predicted by the model when encountering high pressure (see Appendix DEL). The assumptions in the BRAGFLO direct-brine-release model (that is, about permeability, two-phase flow properties, crushed panel height, porosity) match those used in the 10,000-year BRAGFLO and CUTTINGS_S models.~~

~~The WIPP two-phase flow code BRAGFLO is used to simulate the direct brine releases during a drilling intrusion. This code is also used to calculate the 10,000-year flow of brine and gas through the WIPP and surrounding rock. However, a different conceptual model has been constructed to represent the excavated rooms, drift passageways, and the salt pillars between them. This refined mesh, or repository scale model, more accurately captures the flow patterns associated with the short-duration direct releases. The suite of software used to calculate direct brine releases is discussed in Appendix CODELINK. The output from the repository-scale direct release model is the volume of brine (cubic meters) released to the surface. The activity of radioisotopes in the brine released is determined using the actinide source term model.~~

MASS-16.3 Long-Term Properties of the Abandoned Intrusion Borehole

The purpose of the model for the long-term properties of the intrusion borehole is to provide in BRAGFLO the physical properties relevant to fluid flow through a plugged and abandoned borehole that intersects the repository. The model includes several possible plugging and configuration patterns based on current practice in the Delaware Basin (***CCA Appendix MASS,*** Attachment 16-1). Because plugging practice is closely controlled by state regulations, only the New Mexico portion of the Delaware Basin is considered. Section 6.4.7.2 of this application describes the properties assigned to the boreholes and the types of plug configurations considered in performance assessment.

The conceptual model for long-term flow up a plugged and abandoned borehole addresses the principal parameters in the intrusion borehole model for long-term flow: permeability, porosity, compressibility, and two-phase properties. Because these properties may change with time as the borehole plugs degrade, some types of boreholes have several defined stages for the evolution of borehole properties. No retardation of actinides or other transport-limiting effects in the borehole are assumed. ***This is considered a conservative assumption (see Table MASS-1).***

Permeability, the most important borehole property, changes according to the stage of borehole degradation. The values assigned to other parameters are held constant for all stages and are set consistent with a borehole fill referred to as silty sand, consisting of the material that would naturally slough off the walls of the borehole or the remains of degraded plugs. The porosity of the plugged and abandoned borehole is set at a low value within the porosities expected of materials that will be in the borehole; the low value was chosen because smaller void volume in the borehole reduces storage in the borehole and slightly increases the total flux of fluids that may pass through it.

Predictions of the time-dependent permeability of plugged boreholes are based on three configurations for borehole plugs and two concepts of how the plug materials will be altered by fluids. The concepts include steel corrosion and concrete degradation. From the outside inward, the conceptual model for borehole plugs envisions concentric circles of ordinary portland cement as grout attaching the casing to the rock, low carbon steel (the casing), and a central disc of ordinary portland cement (the concrete plug). The bulk of the data used to predict the service lives of borehole plugs comes from the open literature on corrosion of low carbon steel and ordinary portland cement and from tabulated thermodynamic data bases.

Predictions of plug performance derived from the conceptual models are sensitive to both chemical and physical parameters. Key areas of uncertainty include the following:

- opened or closed nature of the physical and chemical systems,
- degree to which performance data from generic materials apply to WIPP-specific materials and conditions,
- conditions at the precise locations where WIPP plugs are emplaced, and
- physical dimensions of the plugs.

The conceptual models for predicting the time-dependent permeability of plugged boreholes recognize two types of systems: open and closed. Open systems are ones in which chemical components can be added or subtracted freely, whereas closed systems are ones in which the identity and amount of chemical components available for reaction are constant. In physical models, a closed system maintains a constant volume, while in open systems volume is unconstrained. The principal area of uncertainty in the conceptual models is the definition of the boundary between open and closed space. This boundary is significant because real systems are somewhere between totally open or closed, and open and closed systems result in very different expected performance lives for plugged boreholes.

In chemical systems, a very small addition or release of reacting components is insignificant, but a substantial change can have large effects: in open systems reactions proceed until the supply of reactants is exhausted. In open systems, equilibrium considerations may have little or no significance; hence treatment by equilibrium thermodynamics may be unenlightening. Similarly, in physical systems, a small amount of system expansion will have little effect on internal stresses, but unlimited expansion may cause the system to fail in tension.

MASS-16.3.1 Corrosion

There are many low-carbon-steel alloys, and not all corrode at the same rate in a given environment. However, because of the aggressive corrosion rate selected for the model, steel composition is not thought to introduce significant uncertainty about the rate. Corrosion of the casing steel has been modeled thermodynamically for plugged boreholes. Hydrogen is a common byproduct of corrosion. An equilibrium hydrogen pressure has been calculated for a number of potential reactions, using metallic iron to represent steel and pure water to represent brines. Attainment of equilibrium hydrogen pressure is taken to indicate cessation of corrosion. To reach equilibrium, the system must contain the hydrogen that is generated. The hydrostatic pressure of the brine column has been assumed to confine hydrogen when the pressure exceeds the equilibrium hydrogen pressure calculated for the corrosion reaction of interest.

Reactions most representative of corrosion of steel casing produce iron hydroxide corrosion products. Equilibrium hydrogen pressures for these reactions are exceeded by hydrostatic pressures at depths greater than about 1,100 ~~feet~~ ***ft*** (335 m~~eters~~). Corrosion of casing above this depth is treated as open; the casing corrodes until the supply of metallic iron is exhausted and the casing disintegrates. Without axial support supplied by the casing, the concrete plug also fails. In contrast, corrosion is assumed to take place in a closed system at depths greater than 1,100 ~~feet~~ ***ft*** (335 m~~eters~~). Hydrogen is not free to nucleate as a gas and leave the system. Although local perforations in the casing are expected, the casing does not disintegrate. It supports the concrete plugs, and permeability changes in the plugs are attributed to alteration of cement phases by the brine that flows through them.

The greatest uncertainty associated with composition is likely to arise from the thermodynamic calculations used in the model. Pure phases (Fe for steel and H_2O for brine) have been assumed so that hand calculations may be more readily performed. Various reactions and environments have been modeled without directly considering complexities in the chemical system (other than volatiles). Qualitatively, the added complexities are likely to have no substantial consequence on the ability of the brines to dissolve a pathway through the casing. However, system complexities might decrease the equilibrium hydrogen pressures calculated for the corrosion reactions or lead to unexpected reaction products.

Data supporting low-carbon-steel corrosion models come primarily from the literature. The empirical data support the assumption that general corrosion is the dominant mechanism for corrosion under oxic conditions and that pitting will occur under low oxygen (and high pH) or elevated carbon dioxide and hydrogen disulfide conditions. Corrosion rates are a function of the conditions under which corrosion occurs. Published data include rates as rapid as 3 ~~millimeters~~ ***mm*** per year, which is the value assumed in the model. Such rapid rates are not inconsistent with reports in the Delaware Basin of casing failures occurring from corrosion within months to years

(***CCA Appendix MASS,*** Attachment 16-3, B-17). Data from corrosion of steel enshrouded in concrete come from the literature on marine construction and the data base on reinforcing steels. These data support the assumption that steel encased in concrete cannot be assumed to corrode more slowly than exposed steel. This subject area is discussed in detail in ***CCA Appendix MASS,*** Attachment 16-3 (Section 3.2 and Appendix B).

MASS-16.3.2 Portland Cement Concrete

The cementitious materials used in hydrocarbon exploration are variable. The degree to which oil-field materials might perform differently from the cement mixtures investigated and reported in the literature is unknown. There is no standard mix formulation that specifies plugging cements precisely; the use of generic data is reasonable, because the vagaries of cement composition are implicitly included. The published empirical studies of concrete degradation include a large body of data for reacting solutions ranging from pure water to marine brines. Waters with higher chloride and magnesium contents cause greater reaction. This level of detail has not been factored into the model directly; rather, alteration by brines has been the favored source when extracting information on degradation.

Chemical alteration of cement phases by brine produces new solids with greater molar volumes than the unaltered, hardened cement phase. In a closed physical system, the alteration will lead to decreased internal porosity and consequent decrease in permeability. In an open physical system, alteration will lead to increased internal pore pressures that will eventually exceed the tensile strength of the concrete plug. The result is often seen on concrete sidewalks or other unreinforced concrete structures: without something to restrain expansion, the concrete cracks, increasing its porosity and permeability.

Current plugging practices create configurations that favor each model. Plugs installed to respond to the New Mexico Oil Conservation Division regulation R-111-P approach 2,000 ~~feet~~ ***ft*** (610 m~~eters~~) in length (State of New Mexico 1988). These plugs are judged to be long enough that they are self-confining. As a result, alteration of R-111-P plugs produces a situation in which performance is indistinguishable from the undisturbed rock. In contrast, plugs emplaced in response to regulations of the U.S. Bureau of Land Management have a mean length near 40 m~~eters~~. This length is judged to be too short to provide self-confinement; alteration of the concrete results in fracturing and increased porosity and permeability in the plug. The plug length that changes the physical system from open to closed is undetermined. For both chemical and physical model elements, a closed system enhances performance.

Simulation of concrete plug degradation follows a model proposed by Berner (1990), in which the matrix degrades after dissolution and removal of soluble materials such as alkali salts. The model is grounded in empirical observations that concrete alteration sequentially removes excess alkalis, portlandite, and tobermorite or calcium-silicate-hydrate (CSH). Decreased strength attends removal of portlandite.

A critical amount of flow must occur before this degradation threshold is crossed. A volume equivalent to 100 pore volumes has been taken as the critical flow volume, based on values for common compositions of ordinary portland cement concrete (Berner 1990). Also following Berner, the model tracks the amount of flow as pore volumes, reasoning that flow occurs only through pores and that alteration is therefore limited to the solids that surround the pores. The model does not explicitly account for the strength of the concrete but instead makes the conservative assumption that physical failure occurs suddenly at the onset of chemical attack on CSH, that is, at approximately 100 pore volumes. As a result, initial porosity of the hardened concrete is a key parameter for timing plug degradation.

The initial permeability of hardened cement is directly related to the connected porosity that permits flow to occur. Initial permeability of ordinary portland cement is a strong function of the water:cement ratio of the mix. Higher water contents produce higher porosity and permeability. To simplify the analysis, ***the CCA used an*** initial plug permeability ~~has been taken as a constant at~~***of*** 5×10^{-17} ~~square meters~~ ***m^2***. This value lies in the upper range of permeabilities reported for ordinary portland cement and is verified by field measurements made during a single field test of borehole plugging conducted for the DOE (***CCA Appendix MASS,*** Attachment 16-3, C-4). ***In their review of the CCA, the EPA required the DOE to treat this parameter as uncertain (EPA 1998b, Section 5.17). DOE implemented log-uniform distribution of values ranging from 10^{-19} to 10^{-17} m^2. This distribution is used for the 2004 PA calculations.***

The initial permeability of the concrete plug is an important parameter because water must penetrate and flow through the structure before it can alter the hardened plug. The lower the permeability, the longer it takes for 100 pore volumes to pass through the plug. Somewhat paradoxically, the lower the porosity, the smaller the volume of water needed before attack of the CSH begins, because the model decouples the relationship between porosity and permeability by holding permeability constant. In the real world, cement formulations with low water:cement ratios generally produce fewer alkalis and have both lower porosities and lower permeabilities. Less water must pass through the concrete body before onset of CSH degradation, but the lower permeabilities lead to a longer life. The simplified model is conservative: it holds the permeability constant at the upper end of the established range while allowing porosity to vary over the full range commonly encountered in ordinary portland cement. This accommodation reflects better knowledge of permeabilities than porosities in as-emplaced borehole plugs. The range in porosity modeled (5 to 40 percent) can create an order-of-magnitude spread in predicted performance life.

Data supporting the concrete degradation model come primarily from two sources: the international repository literature and journals on concrete construction (for example, dams or bridges). The international literature on repositories contains both models and empirical studies confirming that alteration of concrete will result in decreased porosities and permeabilities in closed systems. Experience for dams confirms this conclusion and confirms the diffusion-driven concrete alteration rates used in the model. The general concrete literature confirms the values of initial permeability and porosity of hardened concrete used in the model.

Observations made on cores recovered from potash mines near the WIPP confirm that alteration of concrete plugs is not extensive after decades of service. Qualitative data have been produced by recovery, microscopic inspection, and leach testing of concrete cores recovered from nearby potash mines. These data establish that plugs placed in boreholes will have low initial permeabilities and that plugs placed in the Salado will form tight interfaces at the borehole-rock interface and will not degrade substantially by contact with formation brines in the amounts and compositions that might reasonably be expected. ***See CCA Appendix MASS,*** Attachment 16-3

~~(Section 3.3 and Appendices C and D)~~ ***for the historical discussions of*** ~~discusses~~ concrete ***plug*** alteration ~~of plugs~~ and creep closure of boreholes***.*** ~~in more detail.~~

MASS-16.3.3 Borehole Configurations

The conceptual models for borehole plugs examine three basic possibilities: a continuous plug through the evaporite sequence, a plug below the brine reservoir horizon coupled with a plug between the repository and the Rustler, and three or more plugs with at least one intermediate plug between the brine reservoir and the repository and another between the repository and the Rustler. These possibilities represent simplifications of the plugging schemes documented in ~~the~~***a*** 1996 survey ***during the 1996 CCA and verified by the Delaware Basin Drilling Surveillance Program (see Appendix DATA, Attachment A***~~(see~~ ***; and*** Sections 6.4.7.2.1 through 6.4.7.2.3~~, and Attachments 16-1 and 16-3, Section 2.1~~). ***Since the CCA, plugging data show these three plug configurations continue to represent plugging patterns employed within the WIPP vicinity (WRES 2003, Attachment C).***

As stated, the basis for these assumptions is a detailed survey of plugging practices in the Delaware Basin. The survey examined the lengths, locations, and intervals plugged, as well as the materials used for construction. The locations of plugs are determined partly by stratigraphic changes and partly by operational considerations during exploration and recovery. Variations in plug length and location affect pressure regimes and flow rates through plugs. The 120-~~foot~~ ***ft*** (40-m~~eter~~) length of the plugs is the approximate mean value of approximately 188 plugs in the survey. Minimum lengths prescribed by regulations are 50 ~~feet~~ ***ft*** (15 m~~eters~~) above plus 50 ~~feet~~ ***ft*** (15 m~~eters~~) below casing transitions or recovery points. Additional plug lengths sometimes occur for unspecified reasons. When all else is equal, performance life is proportional to plug length. For conservatism, the model does not consider the longer plugs. In the conceptual model, all plugs are taken to be 120 ~~feet~~ ***ft*** (40 m~~eters~~) long. See ***CCA Appendix MASS,*** Attachment 16-3 (Section 5.0), for a more detailed discussion of plug performance.

The borehole permeability model was assembled beginning in February 1996. Initially, the model considered only the plug configuration stipulated by Oil Conservation Division regulations, but it was subsequently expanded to consider all regulations and practices documented in the New Mexico portion of the Delaware Basin, without specific consideration of their applicability to the WIPP in the future. The model was developed to be straightforward and easy to understand. Use of hand calculations was favored over the use of complex computer codes. As a result, no detailed evaluation of potentially applicable codes was undertaken, and no screening of codes was performed.

~~The text of the attached report (~~***CCA Appendix MASS,*** Attachment 16-3~~)~~ describ***es***~~ing~~ the model and its predictions contains about 40 references with data that support the model. In general, these references support the plug configurations, steel corrosion mechanisms and rates, and concrete alteration processes that underpin the model. ***Additionally, the Delaware Basin Drilling Surveillance Program continuously monitors plugging practices in the WIPP vicinity (WRES 2003).***

MASS-17.*0* CLIMATE CHANGE

The purpose of this model is to allow quantitative consideration of the extent to which uncertainty about future climate may contribute to uncertainty in estimates of cumulative radionuclide releases from the disposal system. Consideration is limited to conditions that could result from reasonably possible natural climatic changes. The model is not intended to provide a quantitative prediction of future climate, nor is it intended to address uncertainty in system properties other than estimated cumulative radionuclide releases that may be affected by climate change. This model is also discussed in Section 6.4.9.

As discussed in ***CCA*** Appendix CLI, paleoclimatic data from the literature form the basis for reconstructing the climatic variability in southeastern New Mexico since late Pleistocene time, spanning the transition from full glacial conditions in North America (ice sheets as far south as the Northern Great Plains) to the present interglacial period. The wettest and coolest climate at the WIPP corresponded to periods of continental glaciation. During Holocene time (the past 10,000 years), the climate has been predominantly dry, like that of the present, with several wetter episodes.

Future climate at the WIPP may differ in the next 10,000 years from that of the present, but it should be bounded by the extremes of the late Pleistocene glaciation. For the purposes of performance assessment, the DOE assumes that uncertainty about future climate is adequately captured by considering two possible patterns: one in which the Holocene pattern of predominantly dry conditions alternating with wetter conditions continues; and one in which the climate becomes continuously wetter.

Effects of climatic change on the WIPP are limited in the performance assessment model to effects on groundwater flow in the Culebra. Flow (that is, specific discharge in the ***MODFLOW-2000*** ~~SECOFL2D~~ model) is increased from its present calibrated value by a sampled factor that ranges from 1.0 to 2.25 to simulate effects of wetter climates. Possible decreases in flow during drier climates are not considered. Justification for limiting the effects of climate change to flow in the Culebra is based on regional three-dimensional modeling that estimates the extent to which changes in recharge will alter the altitude of the water table and in turn affect flow in the Culebra and other units. Maximum recharge rates considered in the analysis result in a simulated water-table altitude at or near the ground surface throughout the region. Other effects of climatic change, including changes in temperature, wind, evapotranspiration, and vegetation, are not modeled explicitly but are qualitatively included in this analysis through the consideration of the effects of varying recharge.

The climate change model is implemented through the use of a single parameter, the Climate Index. This parameter is a dimensionless factor by which the specific discharge in each grid block of the ***MODFLOW-2000***~~SECOFL2D~~ domain is multiplied. It is a sampled parameter in the ~~performance assessment~~ ***PA***, with a bimodal distribution ranging from 1.00 to 1.25 and from 1.50 to 2.25. See Corbet (1995) and ***CCA Appendix MASS,*** Attachment 17-1 for a discussion of this distribution.

The climate change model used for performance assessment is predicated on the assumption that climate will change during the next 10,000 years. The extent of this change is uncertain, but it should be bounded by the changes that occurred in the past during the peaks of Pleistocene glaciation. Other conceptual models for climate change are not consistent with present scientific understanding of the Earth's climate or with the EPA's guidance to consider natural processes of climatic change (EPA 1996, ***pp.*** 5227-5228). For example, climate could be assumed to remain constant for 10,000 years, but this would be inconsistent with scientific understanding of climate. Alternatively, climate could be assumed to change to conditions unlike any known from the Pleistocene; however, no natural processes are known that could result in such change within 10,000 years.

As discussed in Corbet (1995) and ***CCA Appendix MASS,*** Attachment 17-1, the implementation of climate change in the performance assessment incorporates uncertainty about future climates within the range known from the Pleistocene. Alternative approaches to treating climate change in the performance assessment (that is, varying boundary conditions rather than specific discharge) are discussed in the following section. Past analyses performed using a different approach as part of the 1991 and 1992 preliminary performance assessments suggest that disposal system performance is not sensitive to climate change (Swift et al. 1994, ***p.*** 12).

MASS-17.1 Historical Context of the Climate Change Model

See CCA Appendix MASS, Section MASS.17.1 for historical information on the Climate Change model. This Climate Change model is unchanged for the 2004 PA.

~~Past changes in climate at the WIPP have been recognized since the earliest site characterization work. As described in Appendix GCR (3-102), Brokaw et al. (1972) and Bachman (1974) interpreted the sedimentary record of the Gatuña, the Mescalero caliche, and the overlying surficial sediments (see Chapter 2.0, Sections 2.1.3.8, 2.1.3.9, and 2.1.3.10) as indicating alternating wetter and drier climates during the Pleistocene. Bachman continued extensive geologic work in the WIPP region throughout site characterization and further documented the sedimentary evidence for Pleistocene climatic change (Bachman 1976, 1980, 1981, 1985, 1987). One borehole, WIPP-15, was drilled in 1978 in San Simon Sink southeast of the WIPP to examine the causes of subsidence in the sink and to obtain paleoclimatic data (SNL and University of New Mexico, 1981). Core from the borehole indicates about 547 feet (167 meters) of total subsidence in the Quaternary. Aquatic fauna and flora from the upper 98 feet (30 meters) of core indicate a wet climate followed by an arid period before the present.~~

~~In addition to site-specific geologic evidence, past climatic changes have been inferred by other workers throughout the southwest based on various data. Bachman (1989) prepared an annotated bibliography of relevant information published as of 1984. Swift (see Appendix CLI) prepared a synthesis of Pleistocene climate at the WIPP based on detailed examination of available literature. Swift's analysis forms the basis for the DOE's present understanding of climatic change.~~

~~Early interest in the possible effects of climatic change on disposal system performance focused on the possibility that wetter climates might increase rates of salt dissolution. As discussed in Chapter 2.0 (Section 2.1.6.2), and Appendix SCR (Section SCR.1.1.5.1), average dissolution rates over the past several hundred thousand years include both wet and dry climates and are too low to affect disposal system performance during the next 200,000 years. Questions have also~~

~~been raised about whether dissolution or precipitation of fracture fillings in the Culebra could occur during climatic changes and alter the rate of radionuclide transport in groundwater. As discussed in Appendix SCR (Section SCR.1.1.5.2), isotopic data from Siegel et al. (1991, 5-53 to 5-57), Chapman (1986), and Lambert (1987) indicate that mineralogical changes from interactions with groundwater have been minimal during late Pleistocene time in the units above the Salado. Future mineralogical changes that might occur during climate changes are therefore also expected to be minimal.~~

~~Based on their interpretation of uranium isotope activity ratios and other isotopic data from WIPP area groundwater, Lambert and Carter (1987) and Lambert (1991) proposed that climatic change in the past could have had a significant effect on groundwater flow direction. In their interpretation, wetter conditions during the late Pleistocene recharged the Rustler in the vicinity of Nash Draw, with flow occurring to the southeast. Drier conditions of the Holocene (including the present) resulted in no recharge and a gradual shift in flow directions to those observed at present.~~

~~Current understanding of regional groundwater flow is consistent with Lambert and Carter's general observation that flow directions may change with changing climate, but the specifics of their proposal are not supported by regional three-dimensional modeling. Flow in the Rustler during the wet period of the late Pleistocene was probably driven by a higher water table than that of the present and probably followed the local topography from east to west at the WIPP, rather than northwest to southeast. Drier conditions of the Holocene resulted in less, but perhaps not zero, recharge, and the altitude of the water table fell. Flow directions in the Culebra shifted to their present north-to-south direction, reflecting regional topography of the Delaware Basin.~~

~~Early assessments of system performance (for example, DOE 1980) did not consider the possibility that climatic change could affect the transport of radionuclides through its effects on groundwater flow. The 1991 preliminary performance assessment for the WIPP contained the first quantitative analysis of the possible effects of climatic change on radionuclide transport through the Culebra (WIPP Performance Assessment Division 1991, 6-35 to 6-43). The effects were approximated by varying heads along a portion of the northern boundary of a two-dimensional flow model for the Culebra. Heads were varied using a function that resulted in three peaks during the next 10,000 years, separated by periods in which heads were lowered to their present values. The maximum head elevations were prescribed by a sampled parameter that, at its largest value, allowed heads to reach the land surface and resulted in the maximum potentiometric gradient across the domain.~~

~~The 1992 preliminary performance assessment for the WIPP used an approach similar to that of the 1991 analyses (WIPP Performance Assessment Department 1993, 6-11 to 6-19). Sensitivity analyses performed for both the 1991 and 1992 preliminary performance assessments indicated that cumulative radionuclide releases were not sensitive to the variation in heads at the northern boundary, conditional on the other assumptions adopted in the preliminary performance assessments (Swift et al. 1994, 9 – 12).~~

~~Variations in boundary heads were abandoned for this performance assessment because the regional three-dimensional modeling provided the basis for an approach that was better linked to the near-surface processes of infiltration and recharge and that offered more control over~~

~~groundwater flow within the controlled area. The degree to which variations in boundary heads affected flow over the repository in previous analyses was in part determined by the location of the boundaries and their distance from the site. Setting boundary conditions closer to the repository could have had a greater effect on flow over the site. Furthermore, restricting changes in boundary heads to a single location restricted the possibility for changes in flow direction.~~

~~In addition to work performed to address the treatment of climatic change in this application, additional work was performed using the regional three-dimensional groundwater model to examine the validity of approximating three-dimensional flow in the Rustler with a two-dimensional model of the Culebra. This work indicates that within the controlled area essentially all flow out of the Culebra is lateral. This result, documented by Corbet (1995), provides the basis for applying a scaling factor derived from a three-dimensional model to a two-dimensional model.~~

MASS-18.*0* CASTILE BRINE RESERVOIR

The conceptual model for the ***hypothetical*** brine reservoir is included in the performance assessment to estimate the extent to which uncertainty about the existence of a brine reservoir under the waste disposal region may contribute to uncertainty in the estimate of cumulative radionuclide releases from the disposal system. The conceptual model is not intended to provide a realistic approximation of an actual brine reservoir under the waste disposal region: data are insufficient to determine whether such a brine reservoir exists.

The Castile is treated as an impermeable unit in PA and plays no role in the analysis except to separate the Salado from the modeled brine reservoir in the BRAGFLO grid. In human-intrusion scenarios, the hypothetical brine reservoir can be penetrated by an intrusion borehole connecting it to the repository. The amount of brine that can enter the repository from the brine reservoir is important to PA because brine is required for gas generation reactions to proceed and can transport radionuclides in solution, contributing to potential releases.

The properties of the hypothetical brine reservoir defined for PA include: permeability, porosity, pore volume, initial pressure, and various two-phase flow parameters. Values assigned for these properties were chosen to either be consistent with the available data from and analyses of borehole penetrations of brine reservoirs in the region, or to provide a reasonable response in the BRAGFLO model.

The treatment of the brine reservoir for the 2004 PA is different than that used in the 1996 CCA PA. The major changes to the brine reservoir representation were made by the EPA in their 1997 PAVT (EPA 1998b, V-B-14). In the 1997 PAVT, EPA defined new parameter ranges for bulk compressibility and total pore volume. The range of bulk compressibility was based on a reevaluation of field test data from the WIPP-12 borehole following the CCA (Beauheim 1997). Since the total volume of the grid cells used to represent the brine reservoir in BRAGFLO is fixed, the range of total pore volume was set by defining a range of "effective" porosity (pore volume = grid volume × effective porosity). This range of porosity values is not representative of the actual host rock rather it was chosen to produce a

reasonable response in the BRAGFLO model by providing a predefined range of total pore volumes based on the field tests at WIPP-12.

For the 2003 WIPP PA, DOE has implemented this approach by assuming that the productivity ratio (PR) remains constant (2.0051 × 10^{-3} m^3/Pa). The productivity ratio is defined as:

$$PR = V\frac{C_r}{\phi},$$

where V is the grid volume of the brine reservoir (18,462,514 m^3), C_r is the bulk compressibility (2 × 10^{-11} to 1 × 10^{-10} Pa^{-1}), and φ is the effective porosity (0.1842 to 0.9208). The porosity range used in the CRA-2003 PA is slightly modified from that used by the EPA because the fixed-grid volume increased slightly from the volume assumed in the CCA BRAGFLO grid. In this approach, bulk compressibility and effective porosity are directly proportional (Stein 2003a). See Appendix PA, Section PA-4.2, for the details on the implementation in PA.

Basic geologic information about the Castile is given in Section 2.1.3.3. The hydrology of the known brine reservoirs is discussed in Section 2.2.1.2.2. The treatment of the hypothetical brine reservoir in the PA is discussed in Section 6.4.8, which also points to supplementary information included in this recertification application.~~The Castile is treated as an impermeable unit in performance assessment and plays no role in the analysis except to separate the Salado from the brine reservoir, that is important in human-intrusion scenarios. Properties of the brine reservoir, including its permeability, porosity, volume, and initial pressure, are chosen to be consistent with available data from borehole penetrations of brine reservoirs in the region.~~

~~Basic geologic information about the Castile is given in Chapter 2.0 (Section 2.1.3.3). The hydrology of the known brine reservoirs is discussed in Section 2.2.1.2.2. The treatment of the brine reservoir in the performance assessment is discussed in Chapter 6.0 (Section 6.4.8), which also points to supplementary information included in this application.~~

~~The principal parameters used in the brine reservoir model, described in Section 6.4.8, include permeability, porosity, pore compressibility, initial pressure, and two-phase flow properties. These parameters are implemented in the BRAGFLO model and affect the amount and rate of brine flow up an intrusion borehole. Brine flow up a borehole is also affected by conditions in other regions of the BRAGFLO model, including most directly the permeability of borehole-fill material and fluid pressure in the borehole. The volume of the brine reservoir is treated as an uncertain quantity in the performance assessment~~

~~Attachment 18-4 discusses the estimate of the probability of intercepting a pressurized brine reservoir used in BRAGFLO to develop the brine reservoir volumes. The probabilities described in this memorandum are used to determine the cumulative distribution function for the volume of a Castile brine reservoir. According to the method used, there is a 6/32 probability of a 32,000-cubic-meter brine reservoir (the probability of 0 and 1 reservoirs combined), a 10/32 probability of a 64,000-cubic-meter brine reservoir, a 10/32 probability of a 96-cubic-meter brine reservoir, a 5/32 probability of a 128,000-cubic-meter brine reservoir, and a 1/32 probability of a 164,000-~~

cubic-meter brine reservoir. See Chapter 6.0 (Section 6.4.12.6) for additional discussion of the probability of intercepting a brine reservoir.

MASS-18.1 Historical Context of the Castile Brine Reservoir Model

See CCA Appendix MASS, Section MASS.18.1 for historical information on the Castile Brine Reservoir model. The FEIS (DOE 1980) acknowledged the possible importance of Castile brine, based largely on the encounter at ERDA-6. However, it concluded that brine probably was not present beneath the WIPP site, based on geologic structure and available well data (including the absence of brine in WIPP-12, prior to deepening). Scenario development for the FEIS considered brine occurrences, but consequences of a brine reservoir were not modeled explicitly. The presence of brine beneath the repository was considered to be extremely unlikely. No natural pathways connecting any brine reservoir with the repository were thought to be present. Boreholes penetrating the repository and any brine reservoir were assumed to be cased, and any flow from a reservoir would, therefore, have no impact (borehole-casing degradation was not considered).

Spiegler (1982) concluded that brine reservoirs, originally at hydrostatic pressure, formed several million years ago, prior to regional-scale erosion and decrease of overburden. He assumed an original connection of the reservoir to the water table and concluded that reservoirs formed (and were presumably isolated) several million years ago.

Spiegler and Updegraff (1983) concluded that the original brines were sea water, but that release of water from gypsum dehydration could not be ruled out. Popielak et al. (1983) agreed that Castile brines were relict or ancient sea water. They estimated a brine-residence time of about one million years, believing that isolation preceded the latest stage of basin tilting.

Popielak et al. (1983) and Faith et al. (1983), on the basis of analyses of brines from the WIPP-12 and ERDA-6 occurrences, concluded that these two reservoirs are isolated occurrences.

Lambert and Carter (1984) hypothesized that there may have been a Pleistocene connection of the reservoirs to the Capitan Limestone, that is, that the brines were originally fresh water. Using several assumptions, they calculated minimum residence times for WIPP-12 and ERDA-6 brines ranging from 360,000 to 880,000 years on the basis of $^{234}U/^{238}U$ activity ratios.

By the time of the Site and Preliminary Design Validation, Borns et al. (1983) concluded that

- reservoirs formed mainly because of gravity tectonics (in response to density inversion of thick halites and anhydrites),
- the WIPP-12 structure (1 percent strain) took a minimum of 10,000 years to form, and
- gravity tectonics were probably continuing, although at a reduced rate, because of decreased overburden over the past few million years.

The conceptual understanding of the origin of reservoirs did not change between the early 1980s and the time of the DSEIS (DOE 1989) and FSEIS (DOE 1990). Brine reservoirs were (and still are) believed to be isolated occurrences. Based on a Time Domain ElectroMagnetic (TDEM) survey over the repository area, Earth Technology Corporation (1988) estimated that a conductive horizon, which could be interpreted to represent Castile brine reservoirs, underlies portions of the waste-emplacement panels (four out of nine soundings directly over the panels). A recent interpretation of this data set is in Attachment 18-5.

For purposes of numerical modeling, hypothetical brine reservoirs were assumed to be radially symmetrical, with an inner highly-fractured zone of high transmissivity, and an outer (less-fractured) zone of moderate transmissivity. The outer zone is surrounded by an infinitely extending anhydrite matrix, representative of intact (unfractured) Castile. The brine-reservoir model produced double-porosity fluid-flow responses. This treatment implicitly assumes that any borehole intersecting an area underlain by a brine reservoir will produce large amounts of brine; the possibility that boreholes could penetrate the highly fractured reservoir, but miss highly conductive fractures, was not considered.

Assuming that the reservoirs are radial, and based on an areal view of wells penetrating the Castile (some of which did and some of which did not encounter a brine reservoir), Reeves et al. (1991) determined that brine reservoirs could be expected to have radii varying from approximately 2,625 to 10,499 feet (800 to 3,200 meters). Deterministic calculations in the DSEIS and FSEIS assumed that any borehole penetrating the WIPP repository would penetrate a Castile brine reservoir, and that this reservoir could be represented by the estimated characteristics of the WIPP-12 brine reservoir.

There was no fundamental change in the conceptual understanding of brine reservoirs in the December 1992 performance assessment. Performance assessment calculations included gas pressurization of the repository, which was not considered in DSEIS calculations. This pressurization helped delay brine depressurization of the Castile reservoirs. It was estimated that brine underlay 25 to 57 percent of the waste-emplacement panels, with a median of 40 percent. This estimate was based on a contouring of the existing TDEM data, and was implemented as a probability of a given borehole intersecting brine. Any borehole penetrating a reservoir was assumed to produce brine. A broad range of significant reservoir properties (for example, initial pressure, storativity) were sampled probabilistically, without assuming that any reservoir present would be represented by WIPP-12 properties. The WIPP-12 characteristics did, however, fall within the sampled range.

Section 6.4.8 describes the DOE's current model of a fractured Castile brine reservoir, as implemented by performance assessment. The main conceptual change is the idea that, because of the high angle of vertical fracturing in Castile brine reservoirs, many boreholes may penetrate a brine occurrence without penetrating a conductive fracture. Thus, even though the recent interpretation (Attachment 18-5) of the TDEM data suggest that 10 to 55 percent of the waste-panel area may be underlain by one or more brine reservoirs, the probability of a borehole in the panel area encountering brine may be lower. The geostatistical study performed by Powers et al. (Attachment 18-6) indicated an 8 percent probability of a borehole in the panel area encountering Castile brine. This probability is assigned to determine whether deep boreholes are of the E1 or E2 type in the 1996 performance assessment.

MASS-19.0 OPTION D PANEL CLOSURES

The certification decision by the EPA (1998a) included several conditions that the DOE was required to meet. In the first of these conditions, the EPA required the DOE to implement a specific design for the panel closure system referred to as Option D and required the concrete monolith to be constructed using SMC. The DOE had included in the CCA four Options (A-D) for the panel closure design. The Option D design consisted of two components; a large monolith constructed of SMC and keyed into the surrounding DRZ, and an explosion wall constructed of concrete blocks, which is not keyed into the DRZ.

The PA calculations that supported the CCA and the subsequent 1997 PAVT calculations included generic panel closures in the BRAGFLO grid. These generic closures were not representative of the Option D design. Specifically, the Option D panel closures are designed to impede fluid flow (brine and gas) between panels over long-time scales. The generic panel closures included in the 1996 CCA and 1997 PAVT calculations were relatively permeable and allowed gas to flow freely between panels. In the 1996 CCA and 1997 PAVT PA calculations, a drilling intrusion into a single panel generally caused pressures in the entire repository to decrease.

Following the certification of the repository, the DOE updated the modeling of the panel closures in PA so that the mandated Option D design was adequately represented. A new panel closure representation was developed and presented to the Salado Flow Peer Review Panel in May 2002 and again in February 2003. The peer review panel approved the new conceptual models, which included the implementation of the Option D panel closures in the grid (Caporuscio et al. 2003).

In the CCA/PAVT BRAGFLO grid, only two panel closures were represented. For the 2004 PA, however, DOE included an additional set of panel closures. Preliminary tests of the Option D panel closure representation (Hansen et al. 2002) concluded that Option D panel closures were effective at impeding fluid flow between panels on the order of thousands of years, but that given enough time, pressures slowly equilibrated. These results suggest that the effect of a single intrusion event on pressures in other panels depends on the number of panel closures that lie between the intruded panel and the other panels. Therefore, DOE decided to divide the RoR region into two regions separated by a panel closure. This panel closure represents a set of four panel closures to be located between the northern and southern internal extended panels. The south RoR represents panels directly adjacent to an intruded panel and the north RoR represents panels that are farther away from the intruded panel (two sets of panel closures lie in between).

The DOE assumes that the effect of the Option D panel closures will be to impede fluid flow through and around the closures. Only the concrete monolith portion of the closure system is assumed to remain effective over the 10,000-year regulatory period. The explosion wall is assumed to effective only for a brief period during the operational period. The explosion wall and the open drift adjacent to the monolith are represented in the BRAGFLO grid by a column of grid cells with the properties of the waste area (e.g., high permeability) and include creep closure effects. The monolith is represented in the BRAGFLO grid by an adjacent column of grid cells with a length equal to the length of the monolith (7.9 m) multiplied by the

number of panel closures in series and a width equal to the width of the monolith (10 m) multiplied by the number of panel closures in parallel. For instance, in Figure MASS-6, the southern panel closure in the BRAGFLO grid represents a single set of two panel closures (in parallel) that separate a single external panel from the one of the two internal extended panels (9 and 10). The middle panel closure in the BRAGFLO grid represents a single set of four panel closures (in parallel) that separate the internal extended panels from one another. The northern panel closure in the BRAGFLO grid represents two sets (in series) of four panel closures (in parallel) that lie between the northern edge of the waste region and the shafts.

It is assumed in the modeling that the DRZ above the concrete monolith will heal and quickly attain a state of relatively low permeability. However, it is also assumed that if pressures exceed the fracture initiation pressure (~12.5 MPa), DRZ and anhydrite marker bed materials that intersect the waste room can fracture and allow gas or brine to circumvent the panel closures by flowing around the concrete monolith. This possibility is included in the implementation of the panel closures in the BRAGFLO by replacing the concrete monolith material with marker bed material everywhere the monolith intersects and cuts through the marker beds. This implementation is appropriate even at low pressures because the permeability range of the concrete and the marker beds is nearly equivalent. And at high pressures, fracturing is considered in these grid elements allowing fluids to flow, thus simulating the consequence of fractures extending around the monolith.

Additional information on panel closure effects on repository performances can be seen in the BRAGFLO Analysis package (SNL 2003c).

MASS-20.0 SUMMARY OF CLAY SEAM G MODELING ASSUMPTIONS

One of the changes to the repository design since the CCA is the raising of the repository horizon in the southern half of the waste panels. Specifically, Panels 3, 4, 5, 6, and 9 will be excavated at an elevation approximately 2.4 m above the level of Panels 1, 2, 7, 8, and 10, and the operations and experimental areas. This change in horizon will bring the roof of the raised rooms to the level of the Clay Seam G. The change is expected to improve roof conditions and enhance operations and mine safety. The DOE submitted a planned change request to EPA that described the change and presented an argument that the change would have minimal impact on long-term repository performance (DOE 2000). The EPA responded to the change request in a letter (EPA 2000) in which they agreed with the DOE that the effects to long-term performance would be minimal.

As part of the Salado Flow Peer Review in February 2003, the DOE did an impact assessment on the possible effects of the horizon change to PA to better demonstrate the minimal impact of this change on long-term performance. Two possible effects of this change on the results of PA were considered in this assessment.

First, it was considered that the horizon change might influence the creep-closure porosity surface calculated by the code SANTOS and used by BRAGFLO to determine the porosity of the waste rooms. This possibility was considered by simulating creep closure around a WIPP disposal room raised to Clay Seam G (Park 2002). The resulting Clay G porosity surface was

then compared with the original porosity surface, which was used in the CCA. The differences were shown to be so minor that long-term PA would not be significantly altered (Park and Holland 2003).

The second effect that was considered was the possibility that the thickness of the upper and lower DRZ, as represented in the BRAGFLO grid, might change due to the horizon change. Specifically, in the raised part of the repository, the lower DRZ might become thicker since the distance from the floor of the rooms to MB 139 will be greater than in the unraised part of the repository. A similar decrease in the thickness of the upper DRZ might occur as the roof of the rooms would be nearer to MB 138. Since the DRZ is assumed to be an important source of brine in BRAGFLO, these potential changes to the thickness of the DRZ might affect the amount of brine available to the waste in the raised panels. To assess whether such a change would affect long-term performance, DOE ran a single replicate of 100 undisturbed BRAGFLO vectors in which the total pore volume in the DRZ was adjusted to account for the thickness changes (Stein and Zelinski 2003a). Pressure and saturation results within the waste regions were compared to results assuming the original DRZ thicknesses. It was concluded from these comparisons that the effects of the DRZ thickness changes were very minor and not at all significant for long-term repository performance (Stein and Zelinski 2003b).

The results of the impact assessment were presented to the Salado Flow Peer Review panel in February 2003. The panel accepted the position that the repository horizon change was adequately represented by the impact assessment and need not be implemented explicitly in the BRAGFLO grid for PA calculations (Yew et al. 2003). Based on the results of this impact assessment and the acceptance of the Salado Flow Peer Review, the DOE has determined that it is not warranted to include the change in the repository horizon to Clay Seam G explicitly in the BRAGFLO grid.

MASS-21.0 EVALUATION OF WASTE STRUCTURAL IMPACTS, EMPLACEMENT AND HOMOGENEITY

During the development of the CCA PA, the DOE choose to assume random placement of TRU waste in the WIPP, and developed conceptual and numerical models accordingly. The EPA reviewed these models and their results, and determined that DOE had modeled accurately random placement of waste in the disposal system. Since the time of the CCA, additional information about the waste and its emplacement has emerged, and requires the assumption of random placement to be reevaluated. The waste inventory estimates have been updated since the CCA PA (see Appendix TRU WASTE), resulting in different estimates of important waste components, such as CPR materials. Additionally, the CCA PA assumed that all waste could be modeled as if the waste was emplaced in 55-gallon drums. However, the DOE is emplacing waste using several different types of waste containers, including standard waste boxes (SWBs) and pipe overpacks (Section 4.1)). Waste has been shipped to WIPP in campaigns from the generator sites, resulting in waste emplacement that appears inconsistent with the representation of the waste as a homogeneous material. Finally, DOE plans to emplace waste types, such as supercompacted waste, that were not considered in the CCA inventory (DOE 2002). As a result of this new information and these proposed changes, DOE

performed a separate analysis (Hansen et al. 2003a) to determine if the modeling assumptions used in PA continue to adequately represent the waste.

Many important waste characteristics, such as the radionuclide content and the mass of CPR materials, are directly incorporated in PA by means of waste material parameters. These parameters have been updated consistent with the inventory update (see Appendix TRU WASTE) and thus are represented in the 2004 PA. However, PA does not account for heterogeneity in waste materials or in waste containers. At the Idaho National Engineering and Environmental Laboratory, for instance, debris waste will be volume-reduced by supercompaction, resulting in a very dense waste form containing a high concentration of CPR material. In addition, the Pu residues from the Rocky Flats Environmental Technology Site have been packaged in pipe overpacks, which are more rigid than the typical 55-gallon drum assumed in the CCA. Additionally, PA assumes that waste is emplaced in a random or homogeneous manner. Actual waste emplacement is determined by the availability of waste at generator sites and the shipping schedules. Pipe overpacks occupy about 43 percent of the containers emplaced in Panel 1, suggesting that actual emplacement will not be statistically random.

The analysis reported in Hansen et al. (2003a) focused on potential effects of supercompacted waste and of waste in pipe overpacks on repository performance. Both waste types are structurally stiffer than the generic waste model used in the CCA PA, and the supercompacted waste in particular has high concentrations of CPR materials. The analysis began with a systematic reevaluation the baseline FEPs to identify specific components of PA that could be affected by supercompacted waste. The reassessment concluded that the FEPs "screened in" were adequate to represent the variety of waste types and containers, and that none of the "screened out" FEPs should be reconsidered for implementation. The FEPs assessment concluded that creep closure of the repository, chemical conditions of the waste, gas generation models, and waste mechanical properties could be affected by heterogeneities in the waste materials and waste containers. In addition, DOE determined that the assumption of random waste emplacement should be reevaluated.

Analysis of creep closure of waste-filled rooms, accounting for several types of waste materials and packaging, indicated that a wider range of long-term porosities could occur relative to that established in the CCA, given the uncertainties about the structural integrity of waste packages and their spatial arrangement in the repository (Park and Hansen 2003). For this reason, the analysis in Hansen et al. (2003a) treated creep closure as an uncertain variable. Sensitivity analysis showed that this additional uncertainty did not affect the results of PA in a significant way.

Chemical conditions also were reexamined under a range of possible waste arrangements. The assessment found that regardless of actual waste emplacement, the MgO would still be sufficient to maintain desired chemical conditions. Moreover, the constituents of supercompacted waste would not alter the reactions that determine chemical equilibrium and, consequently, no changes to actinide solubilities or to the gas generation models were warranted.

Supercompacted waste contains elevated amounts of CPR materials relative to other waste streams, and the future arrangement of this waste in the WIPP repository is uncertain. Thus, the analysis treated the spatial distribution of CPR materials as uncertain. However, sensitivity analysis demonstrated that uncertainty in the spatial distribution of CPR materials had little effect on PA results.

The representation of the waste properties also was considered; however, it was determined that no changes to permeability, shear strength, or tensile strength were warranted. Based on this evaluation, no changes to the models for direct releases were necessary.

Direct releases as a consequence of a drilling intrusion are calculated with the assumption of random waste emplacement in the repository. In addition, releases by spallings, DBR, and long-term radionuclide transport assume that radionuclides are homogeneously distributed throughout the waste. A sensitivity analysis determined that PA results are not greatly affected by the assumption of random waste emplacement or by the assumption that radionuclides are homogeneously distributed.

Based on the analysis reported in Hansen et al. (2003a), DOE concluded that:

1. ***Explicit representation of the specific features of supercompacted waste and of waste in pipe overpacks, such as structural rigidity, was not warranted in modeling, since PA results were relatively insensitive to the effects of such features.***

2. ***PA results were not affected significantly by the assumption of nonrandom waste emplacement and the representation of these waste types as a homogeneous material.***

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