Sandia National Laboratories
Waste Isolation Pilot Plant

Conceptual Models in WIPP Performance Assessment

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LIST OF ACRONYMS

AP	Analysis Plan
APPA	Additional Panels Performance Assessment
CARD	Compliance Application Review Document
CCA	Compliance Certification Application
CCMPR	Changed Conceptual Models Peer Review
CFR	Code of Federal Regulation
CMPR	Conceptual Model Peer Review
CRA	Compliance Recertification Application
DOE	Department of Energy
DBR	direct brine release
DRZ	disturbed rock zone
EPA	Environmental Protection Agency
FEP	feature, event, and process
PA	performance assessment
PCR	Planned Change Request
PCS	panel closure system
ROM	run-of-mine
WIPP	Waste Isolation Pilot Plant

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1 Introduction

Within the context of the Waste Isolation Pilot Plant (WIPP) performance assessment (PA), a conceptual model is a set of descriptions and assumptions used to define a system or subsystem for a given purpose. At a minimum, these descriptions and assumptions concern the geometry and dimensionality, initial and boundary conditions, time dependence, and the nature of the relevant physical and chemical processes associated with the disposal system. These descriptions and assumptions should be consistent with one another and with existing information within the context of the given purpose (U.S. DOE, 1996, Section 6.4.1).

Conceptual models are derived from features, events, and processes (FEPs) that are deemed important to repository performance. The conceptual models guide the development of mathematical models for the repository system. Mathematical models comprise a set of equations that relate various physical characteristics. Mathematical models are implemented in numerical models that approximate the solution to the mathematical model's equations; calculations are conducted using computational models (codes) that implement the numerical models.

This document describes the conceptual models used in the WIPP PA and documents the history of changes to each conceptual model. The use of italics in this document indicates a quotation. Within this italicized text, slight editorial changes may exist (e.g. removal of citations to tables and figures), however no meaningful content changes occur.

2 WIPP Conceptual Models

According to the WIPP Compliance Certification Criteria at 40 CFR § 194.23, compliance applications must include descriptions of the relevant conceptual models. The Certification Criteria also state that conceptual models must be peer reviewed according to 40 CFR § 194.27. EPA guidance for § 194.23 states that peer review should answer the fundamental question of "Do the final conceptual model(s) and the subsystem components used in the compliance application represent a reasonable approximation of the actual disposal system?" Guidance states that the conclusions of any peer review must be clearly documented and included in compliance certification applications (or recertification applications). Accordingly, documentation of peer reviews of the WIPP conceptual models used in performance assessment was included in the WIPP CCA (U.S. DOE, 1996).

Changes to the disposal system or its sub-elements have been necessary as the WIPP project has progressed through the operational phase. Operational changes or improved scientific understanding can necessitate changes in the conceptual models from their initial peer-reviewed status as presented in the CCA. When these changes occur, the newly proposed or modified conceptual model(s) must again be peer reviewed to determine their continued adequacy in reasonably representing the disposal system (or component of the disposal system). Until these modified conceptual models have successfully been peer reviewed, they may not be used in demonstrations of compliance. Since the CCA, there have been four formally conducted peer reviews. These peer reviews are listed below:

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1) Salado Flow Peer Review (U.S. DOE, 2003a)
2) Spallings Conceptual Model Peer Review (U.S. DOE, 2003b)
3) Waste Isolation Pilot Plant Culebra Hydrogeology Conceptual Model Peer Review (Burgess et al., 2008)
4) Additional Panels Performance Assessment (APPA) Changed Conceptual Models Peer Review (Falta et al., 2021)

In addition to DOE-initiated peer reviews and associated conceptual model changes, the EPA has also required changes, without peer review, to various aspects of PA as a result of their review and approval of compliance documentation submitted by the DOE. These EPA-mandated changes may affect the assumptions, implementation, or parameterization of a conceptual model.

Table 1 below lists each of the 24 WIPP conceptual models and indicates changes that have occurred since the initial certification of the WIPP. The following sections of this report detail each of the 24 WIPP conceptual models, as well as any peer-reviewed or EPA mandated changes that have occurred since the CCA.

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Table 1. Conceptual models for the WIPP performance assessment

Conceptual Model	Description in the CCA (U.S. DOE, 1996)	Conceptual Model Changes Implemented by Peer Reviews or Required by EPA
Disposal System Geometry	Section 6.4.2.1 Appendix PEER 1, Section 3.1.1	U.S. DOE Salado Flow Peer Review (U.S. DOE, 2003a) CRA-2004, Appendix PEER 1, Section 3.1.2 (U.S. DOE, 2004) Additional Panels Performance Assessment (APPA) Changed Conceptual Models Peer Review (Falta et al., 2021)
Culebra Hydrogeology	Section 6.4.6.2	Waste Isolation Pilot Plant Culebra Hydrogeology Conceptual Model Peer Review Final Report (Burgess et al., 2008)
Repository Fluid Flow	Section 6.4.3.2	U.S. DOE Salado Flow Peer Review (U.S. DOE, 2003a) CRA-2004, Appendix PEER 1, Section 3.1.2 (U.S. DOE, 2004) Additional Panels Performance Assessment (APPA) Changed Conceptual Models Peer Review Report (Falta et al., 2021)
Salado	Section 6.4.5	None
Impure Halite	Section 6.4.5.1	None
Salado Interbeds	Section 6.4.5.2	None
Disturbed Rock Zone	Section 6.4.5.3 Appendix PEER 1, Section 3.7.1	U.S. DOE Salado Flow Peer Review (U.S. DOE, 2003a) CRA-2004, Appendix PEER 1, Section 3.1.2 (U.S. DOE, 2004)
Actinide Transport in the Salado	Section 6.4.5.4 Appendix PEER 1, Section 3.8.1	None

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Conceptual Model	Description in the CCA (U.S. DOE, 1996)	Conceptual Model Changes Implemented by Peer Reviews or Required by EPA
Units Above the Salado	Section 6.4.6 Appendix PEER 1, Section 3.9.1	None
Transport of Dissolved Actinides in the Culebra	Section 6.4.6.2.1	None
Transport of Colloidal Actinides in the Culebra	Section 6.4.6.2.2	None
Exploration Boreholes	Section 6.4.7 Appendix PEER 1, Section 3.12.1	None
Cuttings and Cavings	Section 6.0.2.3.1	None
Spallings	Section 6.4.7.1	Spallings Conceptual Model Peer Review (U.S. DOE, 2003b)
Direct Brine Release	Section 6.4.7.1	Additional Panels Performance Assessment (APPA) Changed Conceptual Models (Falta et al., 2021)
Castile and Brine Reservoir	Section 6.4 8	None
Multiple Intrusions	Sections 6.3.2.2, 6.4.12.3, 6.4.13.3, 6.4.13.4 and 6.4.13.5 Appendix PEER 1, Section 3.17.1	None
Climate Change	Section 6.4. 9	None
Creep Closure	Section 6.4.3.1 Appendix PEER 1, Section 3.19.1	None
Shaft and Shaft Seals	Section 6.4.4	Salado Flow Conceptual Models Peer Review (U.S. DOE, 2003a)
Gas Generation	Section 6.4.3.3	None

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Conceptual Model	Description in the CCA (U.S. DOE, 1996)	Conceptual Model Changes Implemented by Peer Reviews or Required by EPA
Chemical Conditions	Appendix PEER 1, Section 3.22.1 Section 6.4.3.4	Technical Support Document for Section 194.23 Review of the 2004 Compliance Recertification PABC (U.S. EPA 2006) CRA-2009, Appendix SOTERM, Section SOTERM-2.4.1.1 (U.S. DOE, 2009) CRA-2014, Appendix PA, Section PA-4.2.5 (U.S. DOE, 2014) TSD for Sections 194.23, 194.32, and 194.33 Review of Changes to WIPP Performance Assessment Features, Events, and Processes in the 2014 CRA (U.S. EPA, 2017) CRA-2019 (U.S. DOE, 2019 Appendix PA-2019, Section PA-1.1.9).
Dissolved Actinide Source Term	Section 6.5.3.5 Appendix PEER 1, Section 3.23.1	None
Colloidal Actinide Source Term	Section 6.4.3.6 Appendix PEER 1, Section 3.24.1	None

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3 Disposal System Geometry

3.1 Description in the CCA

The Disposal System Geometry conceptual model is best described in U.S. DOE (1996), Appendix PEER 1, Section 3.1.1:

> *The Disposal System Geometry conceptual model expresses the dimensionality of the engineered system and surrounding geologic/hydrogeologic formations. The parameters of dimensionality are length, width, and height, which are expressed in individual grid blocks and remain constant for all scenarios and realizations. The processes that rely on the geometric assumptions and parameters of dimensionality are represented across the overall performance assessment system through a finite difference mathematical model called BRAGFLO. The principal processes that depend on the conceptual model for disposal system geometry are fluid flow and actinide transport.*

The conceptual model is also described as part of the peer review completed by Falta et al. (2021):

> *The Disposal System Geometry conceptual model represents the dimensionality of the engineered repository system and surrounding geologic/hydrogeologic formations for the purpose of modeling flow and transport processes. Dimensionality includes physical dimensions of length, width, and height. The Disposal System Geometry conceptual model provides the framework within which features, events and processes deemed important to flow and transport are represented in mathematical, numerical, and computational models.*
>
> *Repository features represented in the Disposal System Conceptual model include: the waste panels comprising the several waste rooms and pillars; drifts; panel closures; non-waste excavated areas; the shafts and the shaft seals. Features of the geologic environment around the repository include the disturbed rock zone (DRZ), the Salado, and the anhydrite Salado interbeds. Features of the regional geologic system include the Castile Formation below the Salado, and the Rustler Formation above the Salado. Features introduced for modeling the effect of intrusions include the borehole and borehole plugs. Details of each feature may vary among the mathematical, numerical, and computational models for different events and/or processes.*

Key assumptions for the Disposal System Geometry conceptual model include:

1) The three-dimensional system can be represented by two-dimensional simplifications, in which volume is represented by assigning a depth to each two-dimensional grid cell.
2) Horizontal convergent or divergent flows in the rock outside of the repository can be represented by the divergent flaring of the two-dimensional grid to the north and south away from the repository.
3) Details of features within the repository such as the waste panels, shafts and panel closures can be represented by simplified features in the computational grid.
4) The entire repository can be represented by the simplified floor plan used in the computational model.
5) The effects on flow and transport of a randomly placed intrusion borehole can be represented by modeling one intrusion at a designated location in the modeling grid.

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6) Convergent or divergent flows within the repository can be represented by the volumetric flaring of grid cells around the borehole feature.

In the computational models for flow and transport, the disposal system geometry is realized by a single computational grid with different maps of material properties. Material property maps change to represent the presence and characteristics of an intrusion borehole, as well as temporal changes in materials over time.

Modelling assumptions that relate to the Disposal Geometry conceptual model as used in the CCA are found in U.S. DOE (1996), Appendix MASS, Section MASS.4.1.

3.2 Changes since the CCA

(Conceptual Model Change) In 2002, during preparation for the 2004 Compliance Recertification Application (CRA-2004), the Salado Flow Peer Review (U.S. DOE, 2003a) considered and concurred with changes to repository modeling which involved the Disposal System Geometry conceptual model. Changes were: 1) Simplification of the shaft seal system within the model, 2) Implementation of Option "D" panel closure design, 3) Dividing the remainder of the repository into two blocks separated by a panel closure, 4) Applying a new method by which flaring is calculated, 5) Refinement of the grid geometry, and 6) Changing part of the repository horizon to correspond with Clay Seam "G".

(Conceptual Model Change)[1] In preparation for a Planned Change Request (PCR) to add replacement and additional waste panels to the WIPP, the Additional Panels Performance Assessment (APPA) Changed Conceptual Models Peer Review (CCMPR) (Falta et al., 2021) considered changes to the Disposal System Geometry conceptual model and the models which implement this conceptual model, to include:

- Blocks of grid cells to represent the additional waste panels and the associated access drifts. The group of nine additional waste panels, and the associated access drifts, are each represented by a single simplified volume. The key aspects preserved by this simplified representation include the total volumes of the additional panels and access drifts, the hydraulic connections between these volumes and the adjacent DRZ, Salado and Salado interbeds, and the presence of panel closures separating each additional panel from the access drifts.
- Placement of the additional waste panel grid cells with the non-waste filled access drifts, operations, and experimental areas interposed between the additional waste panels and the existing waste panels. The separation reflects the expectation that any flow between the two groups of waste panels would be through the non-waste filled excavated volumes rather than through the intact Salado rock.
- The stratigraphic dip (1° southward) is applied to the grid cells representing the additional waste panels and access drifts, although in the 3D analysis these drifts are approximately orthogonal to the southward dip of the excavated repository. This is rationalized by the fact that the western drifts are fully connected with the Experimental and Observation areas.
- The center of regional flaring (a point within the repository volume) is moved to the midpoint between the regions representing the southern and western groups of waste panels. Flaring is not applied to the columns of grid cells with Salado material adjacent to the waste areas, to

[1] These changes are currently pending approval by the EPA.

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improve flow modeling between regions with greatly different permeability and porosity (Falta et al., 2021, Section 3.0).

The peer review found the proposed changes to be adequate and reasonable for their intended use (Falta et al., 2021).

4 Culebra Hydrogeology

4.1 Description in the CCA

The Culebra hydrogeology conceptual model is described in U.S. DOE (1996), Section 6.4.6.2:

> *The Culebra is conceptualized as a horizontal, confined aquifer. For fluid flow, it is conceptualized as a heterogeneous porous medium which is represented by variations in transmissivity. A heterogeneous velocity field is used for transport calculations, but all other rock properties are conceptualized as constant (homogeneous) across the model area. The Culebra is conceptualized as having two types of porosity; a portion of the porosity is associated with high-permeability features where transport occurs by advection, and the rest of the porosity is associated with low-permeability features where advective flow does not occur and retardation occurs by physical processes (diffusion) and chemical processes (sorption). This type of conceptual model is commonly referred to as double-porosity. In this conceptual model, transport and retardation of colloidal particles is also considered. In this section, the principal topic will be fluid flow in the Culebra. The transport and retardation of dissolved actinides will be discussed principally in Section 6.4.6.2.1. The transport and retardation of colloidal particles will be discussed principally in Section 6.4.6.2.2.*
>
> *In the Culebra conceptual model used in performance assessment, the spatial distribution of transmissivity in the Culebra is important. Other potentially important processes acting on Culebra flow and transport are climate change (Section 6.4.9 and Appendix MASS, Section MASS.17) and the effects of subsidence caused by potash mining in the McNutt (Section 6.4.6.2.3 and Appendix MASS, Section MASS.15.4).*
>
> *The conceptual model for the Culebra assumes that fluid fluxes and directions in the future will be the same as they are projected to be at repository closure, unless future mining within the site occurs, in which case changes to fluid flow are calculated. A steady-state flow field is used to represent this assumption. Conditions assumed at site closure are the subsidence effects of mining in the near future outside the site boundary, climate change, and a reasonable estimate of the hydraulic conditions that existed prior to disturbances to the Culebra caused by site characterization activities (see Appendix MASS, Sections MASS.15.4 and MASS.14.2), and Appendix TFIELD, Section TFIELD.2.2).*
>
> *The factors controlling fluid flow in the Culebra are conceptualized to be the hydraulic gradient, transmissivity distribution, and porosity. The hydraulic gradient and transmissivities used in performance assessment are coupled because they are calibrated to observed conditions by a process described in Appendix TFIELD (Section TFIELD.3). Flow fields are calculated with the code SECOFL2D* [Note: MODFLOW has replaced SECOFL2D for the Culebra Flow Calculation] *using an*

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> *assumption of homogeneous porosity in the Culebra. This single value is the total porosity for the Culebra, including both advective and diffusive porosity, as discussed below. Use of a single porosity for the flow calculation does not introduce inconsistency with transport calculations because (1) steady-state flow fields are used so flux through the system is not dependent on porosity, and (2) the velocity of liquid for transport is calculated based on a double-porosity model implemented in the code SECOTP2D. Thus, the important factors for flow calculations are the hydraulic gradient and transmissivity variation.*

The Conceptual Model Peer Review (CMPR), conducted at the time of the CCA, found the Culebra hydrogeology model to be "*inadequate to define variations in the transmissivity of the Culebra at the site scale*" (U.S. DOE, 1996, Appendix PEER 1, Section 3.2.2.5). In the PA conducted for the CCA, Culebra transmissivity (T) fields were produced by "*a numerical model based on extensive hydrogeologic testing*" (U.S. DOE, 1996, Appendix PEER 1, Section 3.2.2.9). The CMPR determined that the Culebra hydrogeology conceptual model's "*inadequacy was inconsequential for performance assessment because an extensive hydrologic data base was developed and serves as an adequate substitute to support numerical modeling*" (U.S. DOE, 1996, Appendix PEER 1, Section 6.0). The numerical model that produced the T-fields used in the CCA relied on measured transmissivities and water levels in nearby boreholes.

The conceptual model for the effects of subsidence caused by potash mining is described along with the conceptual model for Culebra hydrogeology. The occurrence of future mining within the controlled area is represented by the Disturbed Performance Mining Scenario:

> *Consistent with the criteria stated by the EPA in 40 CFR § 194.32 (b), for performance assessment calculations, the effects of potential future mining within the controlled area are limited to changes in hydraulic conductivity of the Culebra that result from subsidence (as described in Section 6.4.6.2.3)* (U.S. DOE, 1996, Section 6.3.2.1).
>
> *Subsidence effects caused by potash mining are included in this performance assessment because of specific criteria in the EPA's 40 CFR Part 194. For incorporating the effects of subsidence caused by mining, the DOE uses the conceptual model provided by the EPA in 40 CFR Part 194 and supporting documents* (U.S. DOE, 1996, Section 6.4.6.2.3).

4.2 Changes since the CCA

(Conceptual Model Change) In 2008, the Revised Culebra Hydrogeology Conceptual Model (RCHCM) peer review was conducted to review the conceptual approach to producing Culebra T-fields. The peer review approved (1) the new methods for the depth-transmissivity relationship and (2) a rationale for the distribution of fracture and vug filling based on the presence of overlying and underlying salt beds (Burgess et al., 2008).

The peer review described the conceptual approach under review as:

> *The objective of the RCHCM is to provide a suite of transmissivity fields (T-fields) for the Culebra that are:*
>
> - *Geologically based,*
> - *Consistent with observed groundwater heads,*

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> • *Consistent with groundwater responses in the Culebra to pumping tests, precipitation, and anthropogenic impacts, and*
>
> • *Consistent with water chemistry*

The peer review concluded that "*the RCHCM* (revised Culebra hydrogeology conceptual model) *is adequate to develop T-fields for application in the site flow model*" although the panel noted three weaknesses in the RCHCM (Burgess et al., 2008, Section 8):

- lack of demonstration of consistency between flow patterns and geochemistry
- lack of consistency between basin-wide and T-field models as related to the method of handling vertical flow
- incomplete understanding of the correlations of depth and evaporite-mineral fracture filling to transmissivity.

5 Repository Fluid Flow

5.1 Description in the CCA

The repository fluid flow conceptual model is described in U.S. DOE (1996), Section 6.4.3.2:

> *Fluid flow modeling within the repository is concerned with (1) fluid flow and distribution in the waste, (2) fluid flow to and from the Salado and shafts, and (3) fluid flow between the repository and intrusion boreholes. These are important in assessing gas generation rates (Section 6.4.3.3), repository pressure, and the mobility of radionuclides in the disposal system. Additional discussion of this topic is provided in Appendix MASS (Section MASS.7).*
>
> *Disposal region fluid flow is affected by the geometrical association of pillars, rooms, drifts, panel closures, possible borehole locations, the time-dependent properties of waste areas resulting from creep closure, flow interactions with other parts of the disposal system, and reactions that generate gas. As described in Section 6.4.3.1, creep closure changes disposal region porosity. Depending on material properties and conditions, brine may flow into the disposal region by moving down shafts and through the DRZ or operations region, or during disturbed conditions, through a borehole. Brine contained in the Salado may flow to the waste disposal region because of pressure gradients created by the excavation. Brine flow into the repository may be reduced as repository pressure increases, and brine may be expelled from the repository if pressure in the repository exceeds brine pressure in the immediately surrounding rock or borehole. Gas may be generated as waste decomposes, causing a pressure increase. Gas may flow away from the waste into lower pressure areas, which may include disturbed areas surrounding the repository, the interbeds, the shafts, or an intrusion borehole. Gas flow into intact, halite-rich rock is not expected because of the expected high threshold pressure of halite (see Section 6.4.5.1).*
>
> *Fluid flow in the disposal system is conceptualized using principles of multiphase flow, except for Culebra flow and transport modeling. In multiphase flow, a residual brine saturation (S_{br}), is defined, which is the minimum saturation at which the brine phase has a nonzero relative*

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> *permeability; below this saturation brine is immobile. In accordance with two-phase flow theory, the residual gas saturation (S_{gr}) in the disposal system corresponds to the gas saturation necessary to create an incipient gas-phase relative permeability; below this saturation waste-generated gas is immobile. The multiphase flow techniques adopted by the DOE are described in Appendix BRAGFLO (Section 4.8).*

5.2 Changes since the CCA

(Conceptual Model Change) In 2002, during preparation for the CRA-2004, the Salado Flow Peer Review (U.S. DOE, 2003a) considered and concurred with changes to repository modeling which involved the Repository Fluid Flow conceptual model. Changes to the original conceptual model are as follows:

1) Brine inflow and outflow rates and gas pressures have potentially been altered by the introduction of the Option "D" panel closure mandated by the EPA.
2) The Disturbed Rock Zone (DRZ) properties have been altered by the allowance of fracturing both in the anhydrite beds and the Salado halite and the "Flow Around" features near plugs at high pressure.
3) The salt creep rate may be affected due to changes in gas pressure.
4) Gas generation is calculated using a different cellulosic molecular weight that provides approximately 10% greater gas production during microbial degradation.
5) Flows will be simplified since the Disposal System Geometry conceptual model now has a simplified Shaft component.

(Conceptual Model Change)[2] The CCMPR considered changes to the implementation of the Repository Fluid Flow conceptual model due to "*the intimate connection between the Repository Fluid Flow and Disposal System Geometry conceptual models*" (Falta et al., 2021, Section 3.0). The peer review found the proposed changes to be adequate and reasonable for their intended use.

6 Salado

6.1 Description in the CCA

The Salado conceptual model is described in U.S. DOE (1996), Section 6.4.5:

> *The Salado is the principal natural barrier to fluid flow between the waste disposal panels and the accessible environment. Fluid flow in natural conditions in the Salado is discussed in Section 2.2.1.3. Excavation of the repository has altered natural pressure gradients in the Salado, creating the potential for fluid flow into the excavation. Fluid flow, gas generation, and volume changes from creep closure cause changes in pressure gradients through time. Salt creep, as well as possible fracturing from high repository pressure, alters the permeability and other flow properties of the rock near the repository. Depending on pressure gradients developed and altered material properties, gas and brine flow may be enhanced in affected portions of the Salado.*

[2] These changes are currently pending approval of RPPCR by the EPA.

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> *For performance assessment, the DOE conceptualizes the Salado as a porous medium composed of several rock types arranged in layers, through which flow occurs according to Darcy's law. Two rock types, impure halite and anhydrite, are used to represent the intact Salado. Once sampled, model parameters for all layers are uniform and constant, with two exceptions, porosity and permeability. Conceptually, this assumption of constant properties is based on observations of compositional and structural regularity in layers exposed by the repository and on the inference that there is little variation in large-scale averages of rock or flow properties across the disposal system. For several meters above and below the repository, a DRZ has increased permeability compared to intact rock and offers little resistance to flow between anhydrite interbeds and the repository. In all rock units, porosity can vary from initial values due to compressibility, depending on pressure changes in a computational grid block. As discussed in Section 6.4.5.2, a model has been implemented in interbeds to simulate the effects of fracturing caused by high repository pressure as pore pressure approaches or exceeds lithostatic.*

6.2 Changes since the CCA

This Salado conceptual model and associated assumptions are unchanged since the CCA.

7 Impure Halite

7.1 Description in the CCA

The impure halite conceptual model is described in U.S. DOE (1996). All halite rocks within the Salado are modeled as impure halite. The impure halite conceptual model:

> *[…] explains the role of impurities in influencing the mechanical and hydraulic properties assumed for the halite-rich rocks of the Salado. The model supports the treatment of the distribution and stratigraphy of impurities in the Creep Closure and Salado conceptual models* (Appendix PEER 1 Section 3.5.1, U.S. DOE 1996).
>
> *The DOE uses a single porous medium with spatially constant rock and hydrologic properties (Region 19 in Figures 6-13 and 6-14) in performance assessment to represent intact, halite-rich layers in the Salado and minor interbeds contained within those layers that are not explicitly represented. A comparison has been made between the simplified stratigraphy used in the performance assessment model and a model with a more detailed stratigraphy in the vicinity of the repository; this comparison supports use of the stratigraphic representation used for performance assessment. This model comparison is described in Christian-Frear and Webb (1996)* (U.S. DOE, 1996, Section 6.4.5.1).

7.2 Changes Since the CCA

This conceptual model and associated assumptions are unchanged since the CCA.

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8 Salado Interbeds

8.1 Description in the CCA

The Salado interbeds conceptual model is described in U.S. DOE (1996), Section 6.4.5.2:

> *Three distinct anhydrite interbeds are modeled: representing MB138, anhydrite layers a and b, and MB139. The three intact interbeds have the same set of model parameters, and the parameters are initially spatially constant. Porosity and permeability can vary spatially during a simulation depending on the extent of interbed fracturing. The interbeds differ only in position and thickness.*
>
> *The three interbeds are explicitly represented because they exist in the disturbed region around the repository within which fluid is expected to be able to flow with relative ease compared to the surrounding formation. MB139 and anhydrite layers a and b are present within the disturbed rock zone (DRZ) that forms around excavations. MB138 is included along with a thick DRZ because of uncertainty in the extent and properties of the DRZ and the associated long-term isolation of MB138 from the repository.*
>
> *In BRAGFLO, brine flows between the Salado and the repository in response to fluid potential gradients that may form over time. Because of the low permeability of the impure halite and relatively small surface area involved, direct brine flow between the impure halite and the repository is relatively small. The interbeds, however, can serve as conduits for brine flow between the impure halite and the repository. Conceptually, brine flows laterally along higher permeability interbeds towards or away from the repository and vertically between the interbeds and the lower permeability halite. Because the interbeds have a very large contact area with adjacent halite-rich rock, even a very small flux from the halite into the interbeds (for brine inflow) or to the halite from the interbeds (for brine outflow) can accumulate into a significant quantity of brine. In this manner, halite serves as a source or sink for brine in the repository.*
>
> *Interbeds contain natural fractures that may be partially healed. If high pressure is developed in an interbed, its preexisting fractures may dilate or new fractures may form, altering its porosity and permeability. Pressure-dependent changes in permeability are supported by experiments conducted in the WIPP underground and in the laboratory (Beauheim et al., 1993). Accordingly, the DOE has implemented a porous-media model of interbed dilation and fracturing that causes the porosity and permeability of a computational cell in an interbed to increase as its pore pressure rises above a threshold value. Model details are presented in Appendix BRAGFLO (Section 4.10) and Appendix MASS (Section MASS.13.3). To the extent that it occurs, dilation or fracturing of interbeds is expected to increase the transmissivity of interbed intervals. The threshold pressure of dilated or fractured interbeds is expected to be low because apertures of the fractures increase; thus, fluid is expected to be able to flow outward readily if adequate pressure is available to dilate the interbeds.*
>
> *The model used to simulate the effects of interbed dilation or fracturing is explained in detail in Appendix BRAGFLO (Section 4.10). In summary, it assigns a fracture initiation pressure above the initial pressure at which local fracturing takes place, and changes in permeability and porosity occur above this pressure. Below this fracture initiation pressure, an interbed has the*

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permeability and compressibility assigned by LHS and representative of intact rock. Below the fracture initiation pressure, the initial sampled porosity is modified slightly with pressure caused by compressibility. Above the fracture initiation pressure, the local compressibility of the interbed is assumed to increase linearly with pressure. This greatly increases the rate at which porosity increases with increasing pore pressure. Additionally, permeability increases by a power function of the ratio of altered porosity to initial porosity. For numerical reasons (that is, to prevent unbounded changes in parameter values that would create numerical instabilities in codes), a pressure is specified above which porosity and permeability change no further.

8.2 Changes since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

9 Disturbed Rock Zone

9.1 Description in the CCA

The disturbed rock zone conceptual model is very generally described in U.S. DOE (1996), Section 6.4.5.3, and more specifically in Appendix PEER 1, Section 3.7.1:

The Disturbed Rock Zone model consists of a description of a fracture zone surrounding excavations that is created by induced stresses. At the WIPP, the primary DRZ exists in all rocks; the secondary DRZ is applicable only in viscoelastic rocks such as halite. The DRZ varies in depth away from the excavation and has been reported to be up to 50 m deep for large excavations. It exists in the repository roof, floor, and walls, and around shaft and borehole walls. Because of the distinctly different stress fields in each of these locations, the DRZ can have different properties at each location. For example, it is considered to disappear under appropriate conditions and with time in the borehole seals program, and is variously applied as it relates to the repository rooms and panels. Related models include Creep Closure, Shafts and Shaft Seals, Disposal Room Geometry, Repository Fluid Flow, Salado, and Salado Interbeds.

Induced changes to the stress field occur immediately on the passage of mining equipment during excavation. In halite, as the salt adjusts to these changes through the creep process, further micro- and macro-fracturing progressively occur in the intact rock, adding to a fracture region known as the DRZ. This DRZ was first technically addressed and demonstrated by Borns et al. (1987, 1988, 1989, 1990). Van Sambeek et al. (1993) have referred to the mining-induced fractures as the initial DRZ and the progressive fracturing as the secondary DRZ. In this analysis, the Panel will not distinguish between these except for their applications. The characteristics of the DRZ include increased rock volume and permeability and decreased brine saturation due to drainage and drying, load bearing capacity, and lithostatic pressure. Clearly these properties could lead to the DRZ providing flow paths for fluids and gases from the repository to those zones that might carry them to the accessible environment. Studies by Munson et al. (1994) have characterized the DRZ and found it to be irregular in thickness and fracturing and able to heal with time under an applied confinement. Two versions of a creep model, applicable to room closure and DRZ development, have been formulated during this period. These are a model that

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includes both transient primary creep and steady state creep (MD model), which has been used in the porosity surface lookup table calculation of repository void space, and the MD model, with added tertiary creep fracture (MDCF), used to confirm DRZ thickness, fracture porosity, and healing characteristics. The MD model is central to the porosity surface calculation (SANTOS), which relates creep, waste compaction, and gas pressure to overall room closure rate. The DRZ is not considered in room closure calculations since all DRZ fracture porosity is assumed to be recovered by healing at final closure. For the waste room, the DRZ model is incorporated by assuming a high permeability and low porosity, with the result that the DRZ is unable to act as a constraint to brine or gas flow from the repository rooms and is unable to store brine. A primary reason for this approach is the uncertain behavior of the rock zone, which is dependent on many uncontrollable factors.

9.2 Changes since the CCA

(Conceptual Model Change) In 2002, during preparation for the CRA-2004, the Salado Flow Peer Review (U.S. DOE, 2003a) considered and concurred with changes to repository modeling which involved the Disturbed Rock Zone conceptual model. During their PAVT sensitivity study, the EPA mandated a range of permeability for the DRZ which reasonably represented the properties of extensively creep-damaged halite and anhydrite at the high-permeability end, and of minimally damaged halite at the low-permeability end. This range was retained in the changed conceptual model and was not previously peer reviewed (Hansen and Leigh, 2003).

10 Actinide Transport in the Salado

10.1 Description in the CCA

The conceptual model for actinide transport in the Salado is briefly described in U.S. DOE (1996), Section 6.4.5.4, but described in more detail in Appendix PEER 1, Section 3.8.1:

The only transport mechanism that will be used in this conceptual model is advection. The Actinide Transport in the Salado conceptual model previously addressed three mechanisms: 1) advection (transport with bulk flow of liquid); 2) dispersion (liquid velocity differences while moving through pores or surface irregularities); and 3) diffusion (molecular motion in presence of concentration gradients). These mechanisms are all standard contaminant transport phenomena. DOE assumed that these three transport mechanisms of actinides in brine represented the most important processes of actinide movement in the Salado Formation. All three mechanisms look at the transport of dissolved or colloidal actinides through the anhydrite interbeds (MB 138, MB 139, and anhydrite interbeds a and b).

Three physical influences that may affect actinide transport in the interbeds have been left out of the conceptual model by DOE to promote a conservative philosophy. These influences are sorption of dissolved actinides on clays, retardation of colloidal actinides by surface features, and mineral precipitation containing trace actinides from brine. Sorption of actinides onto clay surfaces is a known reaction, and DOE is highly confident that it will occur; however, the model conservatively neglects the effect. With regard to retardation of colloidal actinides by surface

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features, it is assumed that offsetting interactions will occur. The philosophy is that colloids can be retarded by surficial features, but will travel faster than the average velocity of the bulk liquid. Precipitation of minerals as brines move into the interbeds due to chemical gradients is a possibility. Given the concept that the amount of precipitation will be minor, and that actinides will only occur in trace amounts in the crystal structures, DOE has decided to neglect this effect in the performance assessment.

Three other mechanical processes may have a lesser impact on actinide transport in the Salado. These are fracture flow, channeling, and viscous fingering. Fracture flow is accounted for in the Salado Interbed model and takes into account increased porosity and permeability through fracture propagation and dilation. DOE expects that other fracture processes and effects not taken into account in the fracture model will be negligible. One process not incorporated, channeling, has offsetting effects. Channeling is the fluid movement through large apertures of a fracture network (i.e., locally high permeability). DOE believes this mechanism will be negated for two reasons. First, if gas is present in the undisturbed state, it will preferentially occupy areas of high permeability over brine. This will preclude these regions of fast transport from brines. Second, the incoming brine will be miscible with the interbed brine. Such miscibility will allow diffusion and mixing phenomena to broaden finger fronts (i.e., reduce concentration gradients) until they are indistinguishable from the advancing brine front.

Gases may also penetrate interbed brines as a fingered front. However, such a mechanism will not affect actinide transport because the actinides of interest are only incorporated in the liquid phase. DOE also assumes that a liquid will not displace gases in the high-permeability regions (channels) due to capillary effects.

10.2 Changes Since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

11 Units Above the Salado

11.1 Description in the CCA

Units above the Salado include, in order from lower to higher, the Los Medaños Member of the Rustler Formation, the Culebra Dolomite Member, the Tamarisk Member, the Magenta Member, the Forty-niner Member, the Dewey Lake Formation, and the units above the Dewey Lake. At the time of the CCA, the Los Medaños Member had not yet been formally named and was referred to simply as the unnamed lower member. For consistency, that terminology is retained in this document.

The conceptual model for units above the Salado defines the hydrogeologic properties that govern flow and actinide transport in these units. A fundamental assumption in the conceptual model for units above the Salado is that lateral actinide transport through these formations within the next 10,000 years is possible only in the Culebra U.S. DOE (1996), Section 6.4.6. As a consequence, the conceptual models for Culebra hydrogeology and for actinide transport in the Culebra are described separately.

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11.1.1 The Unnamed Lower Member

In performance assessment, this member is treated as impermeable, which prevents liquid flow and actinides from entering this unit. The DOE assumes that because of the low permeability of the unnamed lower member, any brine entering it adjacent to an intrusion borehole would be contained well within the site boundary for more than 10,000 years. Therefore, this treatment is conservative, regarding estimated releases into the Culebra, because allowing flow from a borehole or shaft into the unnamed lower member would, if anything, decrease flow into the Culebra. This would have a tendency to reduce the release of actinides from the Culebra to the accessible environment. In performance assessment, the thickness of the unnamed lower member is 118 feet (36 meters), and its permeability is zero (U.S. DOE, 1996, Section 6.4.6.1).

11.1.2 The Tamarisk

In performance assessment, this member is treated as impermeable. This may cause an increase in flow through the adjacent Culebra and Magenta. This treatment is considered conservative in that allowing flow from the intrusion borehole or shaft into the Tamarisk would, if anything, decrease flow into the Culebra, which would tend to reduce the consequence of radionuclide release to the Rustler. In performance assessment, the thickness of the Tamarisk is assumed to be 81.4 feet (24.8 meters) and its permeability is effectively zero (U.S. DOE, 1996, Section 6.4.6.3).

11.1.3 The Magenta

Transport of actinides through the Magenta to the accessible environment is not modeled. The assumption that no releases will occur from the Magenta is based on the hydraulic test results from wells on the WIPP site (Beauheim, 1987, 110-118) that indicate that the Magenta is a porous medium with no hydraulically significant fractures (in contrast to the Culebra) and that its conductivity is lower than that of the Culebra. Early numerical simulations of flow and transport in the Magenta suggested much slower transport than in the Culebra (Barr et al. 1983, 26-27). Therefore, no radionuclides entering the Magenta will reach the accessible environment boundary within the 10,000-year time frame. Accordingly, the BRAGFLO model geometry reasonably approximates the effects of Magenta flow. The Magenta permeability is chosen conservatively as the lowest of measured values near the center of the WIPP site, in order to yield a lower reasonable amount of brine (and radionuclide) storage within the Magenta, while continuing to yield an upper bounding flow into the Culebra (U.S. DOE, 1996, Section 6.4.6.4).

11.1.4 The Forty-niner

As with the Tamarisk and unnamed lower member, the Forty-niner is assigned a permeability of effectively zero in performance assessment. This treatment is considered conservative in that allowing flow from the intrusion borehole or shaft into the Forty-niner would, if anything, decrease flow into the Culebra, which would tend to reduce the consequence of radionuclide release to the Rustler. Its modeled thickness is 56.8 feet (17.3 meters) (U.S. DOE, 1996, Section 6.4.6.5).

11.1.5 The Dewey Lake

Release of actinides to the accessible environment from transport in the Dewey Lake is assumed not to occur even if contaminated brine reaches the unit because the sorptive capacity of this unit appears large. This assumption is based on an analysis (Wallace et al., 1995) that

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demonstrated that the potential sorption capacity of the Dewey Lake is sufficient to prevent releases for 10,000 years. This analysis consisted of (1) a literature review of sorptive capacity of redbeds and (2) an estimate of the minimum sorption required to prevent release of actinides that enter the Dewey Lake to the accessible environment in 10,000 years. Comparison of the sorption values for the Dewey Lake analogues established by literature review with the minimum sorption required to prevent release indicates that the likely sorptive capacity of the Dewey Lake is orders of magnitude greater than would likely be required to prevent release. Therefore, the DOE assumes that chemical retardation occurring in the Dewey Lake will prevent release within 10,000 years of any actinides that might enter it (U.S. DOE, 1996, Section 6.5.6.6).

11.2 Changes since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

12 Transport of Dissolved Actinides in the Culebra

12.1 Description in the CCA

The conceptual model for transport of dissolved actinides in the Culebra is described in U.S. DOE (1996), Section 6.4.6.2.1:

Actinides may be introduced into the Culebra by brine flowing up a borehole or by brine flowing up the shaft. Three principal processes have been demonstrated to occur naturally that affect the transport and retardation of dissolved actinides. Dissolved actinides will be carried by advection in the natural flow of Culebra groundwater. Dissolved actinides will diffuse into the matrix. Dissolved actinides will sorb to varying extents onto the different minerals lining pore walls or fractures. It is possible that dissolved actinides may participate as trace constituents in reactions between water and rock and be bound up in newly formed minerals, but this phenomenon is not included in the conceptual model. These processes are complicated to characterize because of known stratigraphic variation in the Culebra and expected heterogeneity in solution chemistry along the possible flow paths from the injection point to the accessible environment.

The Culebra at the WIPP site is conceptualized as having very low permeability in the upper approximately 9.8 feet (3 meters), and variable permeability in the lower portion, which can be lower than the upper portion in regions where the Culebra as a whole is relatively impermeable. Thus, the bulk of the data indicates that the majority of the flow and transport takes place in the lower portions of the Culebra. Accordingly, for flow and transport calculations, an effective thickness of the Culebra of 13.1 feet (4 meters) is assumed.

There is considerable variability in the structure and size of porous features in the Culebra, including fractures (of a variety of dimensions and interconnectedness), vugs, interparticle and intercrystalline porosity. The principal flow occurs within those features with the high permeability, and slower flow and diffusion are primary processes in the lower permeability features. Tracer test interpretations indicate that at some locations flow occurs predominantly through fractures (advective porosity is low) and at other locations slower transport indicates that flow is occurring in other permeable features such as vugs connected by microfractures, and

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possibly interparticle porosity (higher advective porosity). Tracer test interpretations also indicate that matrix diffusion is an important process in high-permeability regions of the Culebra. In other words, at least two scales of porosity are needed to reasonably represent the transport processes in the Culebra (that is, a double-porosity model). At some locations of low permeability, fractures may be absent or filled with gypsum. An alternative conceptual model for transport at these locations is uniform single porosity with a high porosity. To simplify calculations, the uniform single porosity model was not implemented; the double porosity model implemented results in faster transport.

The processes that occur in the advective porosity portion of the Culebra are advection (flow), dispersion (spreading caused by heterogeneity), diffusion within the advective porosity, and diffusion into the diffusive porosity. Important factors in this conceptual model are the velocities of fluid in the advective porosity, free-water diffusion coefficients, and dispersion coefficients. The most important factor is the fluid velocity. Free-water tracer diffusion coefficients are specified for actinides. Dispersive spreading at the scale of disposal-system modeling is dominated by the effects of heterogeneities explicitly incorporated in the transmissivity fields input to SECOFL2D [Note: SECOFL2D has been replaced with MODFLOW].

Chemical retardation of dissolved actinides is conceptualized to occur by sorption onto dolomite grains exposed in diffusive porosity because of the large amount of dolomite present in the Culebra. Chemical retardation increases if diffusive porosity is smaller because there is a larger volume of rock for sorption. Although clay minerals are present and would sorb actinides in the Culebra, their effects are not included in the conceptual model or parameter values specified. Effective properties for the rock matrix, which is assumed to be homogeneous, and solution chemistry are assumed and are incorporated directly in specification of the parameters for the retardation model (see Appendix MASS, Section MASS.15.2, and Appendix PAR, Parameters 49 through 57).

In summary, the conceptual model for dissolved actinide transport includes the following: transport in advective porosity, physical retardation (diffusion) into diffusive porosity, chemical retardation (sorption) in diffusive porosity, homogeneous rock properties, and a linear isotherm to describe the sorption process. Some of the more important parameters are advective porosity, diffusive porosity, tortuosity, matrix block length, molecular diffusion coefficients, Kd, and the grain density of dolomite in the Culebra.

12.2 Changes since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

13 Transport of Colloidal Actinides in the Culebra

13.1 Description in the CCA

The conceptual model for transport of colloidal actinides in the Culebra is described in U.S. DOE (1996), Section 6.4.6.2.2:

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

The primary distinction in the transport behavior of the different colloidal particles is whether particles diffuse into the matrix from fractures. This is controlled by the difference between the size of colloidal particles and the mean pore-throat diameters in the diffusive porosity of the Culebra. Colloidal particles that are smaller than the pore throats can diffuse into the diffusive porosity. Actinide intrinsic colloids and humic materials are small enough for this to occur. The conceptual model for these particles includes the processes of advection, diffusion, and dispersion in the advective porosity, diffusion into diffusive porosity, and sorption of actinides in diffusive porosity. This model is analogous to the model specified for dissolved actinides, although the parameter values are different. The conceptual model assumes that other retardation processes (for example, filtration) will not occur for actinide-intrinsic colloids and humic materials.

In contrast, colloidal particles that are larger than pore throats will be excluded from the matrix and will remain in advective porosity. Microbes and mineral fragments are conceptualized as being larger than the mean pore-throat diameter in Culebra diffusive porosity. The conceptual model for these particles includes the processes of advection in advective porosity and filtration by small-aperture features that occur within the advective porosity. See CCA Appendix MASS (Section MASS.15.3 and MASS Attachment 15-9) for additional discussion.

Experiments have demonstrated that mineral fragments and microbes are attenuated so effectively by the advective porosity in the Culebra that it was deemed unnecessary to include those colloids in performance assessment calculations. Under the neutral to slightly basic geochemical conditions expected in the Culebra, humic substances were found to not influence the sorption behavior of dissolved actinides. Therefore, actinides associated with humic substances were treated as dissolved species in the performance assessment calculations. The only actinide-intrinsic colloid found to exist in significant concentrations was the Pu(IV)-polymer. At the WIPP, the total amount of Pu(IV)-polymer introduced to the Culebra was found to be insignificant with respect to the EPA normalized release limit and so was not included in transport calculations. See Appendix SOTERM (Section SOTERM.6) and Appendix MASS (Section MASS.15.3.1) for details. See Appendix MASS (Section MASS.15.3.3) for alternative modeling approaches considered.

Indigenous microbes, humics, and mineral fragment colloids in the Culebra may react with actinides introduced to the Culebra in dissolved form to create new colloidal actinides. Newly formed actinide-bearing microbial and mineral colloids, however, will be attenuated similarly to colloidal actinides introduced from the repository. Therefore, disregarding the impact of newly formed microbial and mineral fragment colloidal actinides is conservative. Experimental results

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indicate that humics do not interact with dissolved actinides under Culebra geochemical conditions. Consequently, the quantity of newly formed humic actinides will be insignificant.

13.2 Changes since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

14 Exploration Boreholes

14.1 Description in the CCA

The conceptual model for exploration boreholes is briefly described in U.S. DOE (1996), Section 6.4.7, but more succinctly described in Appendix PEER 1, Section 3.12.1:

> *The Exploration Borehole conceptual model addresses drilling locations, methods, and frequencies within the WIPP controlled area, borehole sealing, and long-term fluid flow through the sealed borehole. Short-term flow through the unsealed borehole is addressed in the Direct Brine Release conceptual model. The Exploration Borehole conceptual model is limited to a single borehole penetrating the repository. The Multiple Intrusion conceptual model describes conditions when more than one borehole is assumed to penetrate a waste panel.* [Appendix PEER 1, Section 3.12.1, U.S. DOE, 1996]
>
> *An exploration borehole may be drilled on the WIPP site for natural resources investigation and may by chance penetrate a waste panel in the repository. Such boreholes are assumed to be drilled by individuals who have no knowledge of the buried waste, after active institutional control of the site has ceased. The conceptual model for exploration boreholes is based in large part on proscriptive requirements of EPA 40 CFR 194. The EPA requirements are paraphrased as follows:*
>
> - *The regulatory time frame is the time period beginning at disposal and ending 10,000 years after disposal [40 CFR 194.21].*
> - *Both deep drilling (to or below a depth of 2,150 feet) and shallow drilling (less than a depth of 2,150 feet) that may potentially affect the disposal system during the regulatory time frame are assessed [40 CFR 194.33(a)]. The approximate depth of the repository is 2,150 feet.*
> - *Exploratory drilling is assumed to be inadvertent and intermittent [40 CFR 194.33(b)(1)].*
> - *Exploratory drilling for those resources provided by the waste in the disposal system or the engineered barriers designed to isolate such waste need not be considered [40 CFR 194.33(b)(1)].*
> - *Drilling events in the Delaware Basin are assumed to occur at random intervals in time and space during the regulatory time frame [40 CFR 194.33(b)(2)].*
> - *The frequency of deep drilling within the WIPP controlled area is assumed to be the sum of the rates of deep drilling for each resource in the Delaware Basin over the past 100 years [40 CFR 194.33(b)(3)].*

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- *The total rate of shallow drilling at WIPP is assumed to be the sum of the rates of shallow drilling for each resource in the Delaware Basin over the past 100 years; however. In considering the historical rate of all shallow drilling, the DOE may, if justified, consider only the historical rate of shallow drilling for resources of similar type and quality to those in the controlled area [40 CFR 194.33(b)(4)].*
- *Future drilling practices and technology are assumed to remain consistent with practices in the Delaware Basin at the time the CCA is prepared, including the types and amounts of drilling fluids; borehole depths, diameters, and seals; and the fraction of boreholes that are sealed [40 CFR 194.33(c)(1)].*
- *Natural processes are assumed to degrade or otherwise affect the capability of boreholes to transmit fluids over the regulatory time frame [40 CFR 194.33(d)(2)].*
- *The effects of techniques used for resource recovery following drilling need not be considered [40 CFR 194.33(d)]*

In developing a conceptual model that incorporates these assumptions, DOE has considered the following:

- *Shallow boreholes will not intercept or affect the integrity of the repository and therefore need not be considered.*
- *Present drilling practices include the relative economic value of the target resource; on this basis, the objectives of exploration drilling at the WIPP site are assumed to be oil and gas because these are the only commercially viable resources for which exploration drilling would occur to or below the depth of the repository horizon.*
- *Although commercially viable reserves of potash are known to be within the WIPP controlled area, inadvertent penetration of the repository during exploratory drilling for this resource was not considered because such reserves lie above the repository depth.*
- *The frequency of deep borehole drilling is estimated based only on historical frequencies of drilling for resources of similar type and quality to those found at the WIPP site.*

[…] All exploratory boreholes are assumed to be drilled in search of hydrocarbon resources and all are therefore assumed to penetrate entirely through the Salado and Castile Formations. […] [3]

Drilling is assumed to be conducted by standard rotary methods. At the time of repository penetration, the borehole is assumed to have been cased to the bottom of the Rustler Formation, following current standard practices. After drilling has progressed through the salt section, an intermediate casing is installed to the bottom of the Castile. Below that depth a third, final production casing is installed, which typically extends to the ground surface during production, but is only cemented near the production zones. On abandonment, the production casing is commonly cut above the cemented zone and reclaimed (Thompson et al. 1996). Fluid and solids that flow through the open borehole immediately on repository penetration are described in the aforementioned Direct Brine Release, Cuttings/Cavings, and Spallings conceptual models. Long-term fluid flow through the sealed borehole is described in the following paragraphs.

[3] This paragraph has been modified from that in Appendix PEER 1, Section 3.12.1 to remove values of parameters specific to the CCA, since such parameters change annually due to the collection of new drilling activity, or the occurrences of pressurized brine encounters in the area surrounding the WIPP.

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On abandonment, three different scenarios have been adopted by DOE to describe the range of current borehole plugging practices. These are (1) a single, continuous cement plug extending from the top of the Salado to the bottom of the Castile; (2) two 40-m cement plugs, one at the bottom of the Castile (top of the Bell Canyon) and one at the bottom of the Rustler; and (3) three 40-m cement plugs, consisting of the two plugs described above plus an additional plug near the Salado/Castile contact below the repository. In addition, all boreholes have approximately 15-m long concrete surface plugs (Thompson et al. 1996).

Degradation of the plugs generally follows the scenarios and rationale presented by Thompson et al. (1996). The continuous plug is not considered to degrade over time because of its structural integrity and the very low brine flow through it. The surface plug is also not considered to degrade over time because of the lack of physical or chemical stresses in the near-surface environment. In the two- and three-plug scenarios the steel casing in the Salado and Castile is expected to be locally pitted and leak within a few decades after abandonment. In these scenarios, within 200 years after abandonment the 40-m concrete plug and remaining casing above the repository and the open casing below the repository are assumed to fail completely from both mechanical and chemical stresses. Simultaneously, with the exception of the concrete plugs below the repository, the entire borehole is assumed to be filled with degraded concrete, corrosion products, and sloughed native materials that are assigned the hydraulic properties of silty sand in accordance with regulatory guidance. Because of increased stresses and halite creep rates below the repository, the borehole filling below the repository is subsequently assumed to be compacted, with a concurrent decrease in permeability. The cement plugs below the repository, however, are assumed to maintain their integrity for the duration of the 10,000-year regulatory time frame because degradation rates will be significantly reduced due to a less aggressive chemical environment. Long-term brine flow is expected to occur to or from the repository through the degrading upper borehole plugs as a function of brine availability and repository pressure.

For long-term flow, the borehole is assumed to be plugged immediately after repository penetration by randomly selecting one of the three plugging scenarios in accordance with its probability of occurrence. The borehole plugs are degraded according to the following assumptions. The continuous plug, the surface plug, and the 40-m plugs below the repository will maintain their initial permeability […] *throughout the 10,000-year regulatory time frame. The 40-m plug above the repository maintains its initial permeability* […] *for 200 years. The borehole between the plugs is assumed to remain open during this period* […]*. The casing is not specifically addressed in the long-term flow model and is assumed to not be present. After 200 years, the upper 40-m plug is assumed to fail and the entire borehole between plugs is assumed to have filled with a material with the properties of silty sand* […]*. The porosity of all borehole materials is held at a constant* […] (U.S. DOE, 1996, Appendix PEER 1, Section 3.12.1).[4]

14.2 Changes since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

[4] This text has been modified from that in Appendix PEER 1, Section 3.12.1 to remove values of parameters specific to the CCA, and implementation details regarding pore compressibility and two-phase flow modeling.

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15 Cuttings and Cavings

15.1 Description in the CCA

Cuttings are solid materials removed by drill bits, and cavings are solid materials eroded from the borehole wall and brought to the surface in the circulating drilling fluid. The cuttings and cavings conceptual model is generally described in U.S. DOE (1996), Section 6.0.2.3.1:

> *In a rotary drilling operation, the volume of material brought to the surface as cuttings is the cylinder defined by the thickness of the unit being drilled and the diameter of the drill bit. The quantity of radionuclides released as cuttings is therefore a function only of the activity of the intersected waste and the diameter of the intruding drill bit. Like all parameters that describe future drilling activities, the diameter of a drill bit that may intersect waste is speculative. The DOE uses a constant value of 12.25 inches (0.311 meters), consistent with bits used at the WIPP depth in the Delaware Basin today. The activity of the intersected waste may vary depending on the type of waste intersected, and the DOE considers random penetrations into remote-handled (RH)-TRU waste and each of the 569 different waste types identified for contact-handled (CH)-TRU waste.*
>
> *The volume of particulate material eroded from the borehole wall and brought to the surface as cavings may be affected by the drill bit diameter, the effective shear resistance of the intruded material, the speed of the drill bit, the viscosity of the drilling fluid and the rate at which it is circulated in the borehole, and other properties related to the drilling process. The most important of these parameters, after drill bit diameter, is the effective shear resistance of the intruded material. In the absence of data describing the reasonable and realistic future properties of degraded waste and backfill, the DOE has used conservative parameter values based on the properties of fine-grained sediment. Other properties are assigned fixed values consistent with current practice.*

U.S. DOE (1996), Appendix PEER 1, Section 3.13 also provides additional details on the Cuttings and Cavings conceptual model:

> *The Cuttings/Cavings conceptual model describes releases during drilling of exploration boreholes. It is one of several models that address the calculation of direct waste release to the ground surface if an exploration borehole inadvertently penetrates a waste panel, creating a possible pathway for transport of waste to the surface. Other associated models include those describing Exploration Boreholes, Repository Fluid Flow, Multiple Intrusions, and Spalling.*
>
> *Of the possible pathways for release during the regulatory time frame, one of the most important is that caused by the inadvertent penetration of a waste storage room by an exploratory borehole. Normal oil and gas drilling practices can provide a means for waste to be released to the ground surface in the circulating drilling fluid (mud). From this intrusion, three mechanisms used by WIPP for waste movement are cuttings, cavings and spallings. Cuttings are waste particles released into the mud from the cutting action of the drill bit itself and from mechanical friction. Cavings are waste particles released by erosion of the borehole walls due to circulating drilling fluids. Spallings are those particulate materials removed and transported by the movement of gases.*

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The cuttings mechanism is the easiest to address because the volume of waste cuttings is a simple product of the borehole cross sectional area times the room height, and is equal to the waste volume produced by the drill bit moving through the waste. Cavings is somewhat more complicated as it must incorporate the erosional effects of the shearing action of the drilling mud as it moves up the borehole annulus. This shearing may be caused by either turbulent or laminar flow. Repository pressure can have effects on cavings, which is covered by the spalling process.

Releases of cuttings and cavings are calculated using analytical equations governing erosion by flow up through the hole bored in the waste room, based on laminar and turbulent flow (Berglund 1992) as implemented by the CUTTINGS_S code. This code calculates the final caved diameter of the borehole that passes through the waste by using appropriate input based on assumed physical properties of the waste and drilling parameters.

15.2 Changes since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

16 Spallings

16.1 Description in the CCA

The spallings conceptual model is generally described in U.S. DOE (1996), Section 6.0.2.3.2:

Unlike releases from cuttings and cavings, which will occur with every borehole intrusion, spalling releases will occur only if pressure in the waste-disposal region exceeds the hydrostatic pressure in the borehole. At lower pressures, below about 8 megapascals, fluid in the waste-disposal region will not flow toward the borehole. At higher pressures, gas flow toward the borehole may be sufficiently rapid to entrain particulate waste. If spalling occurs, the volume of spalled material is affected by the physical properties of the waste, specifically its tensile strength and particle diameter. As is the case for the effective shear resistance for the waste, WIPP-specific experimental data are not available to support parameter values for the tensile strength and average particle diameter of degraded waste and backfill. The DOE has based the parameter values used in the performance assessment on reasonable and conservative assumptions.

The quantity of radionuclides released as spalled material depends on the volume of spalled waste and its activity. Because spalling may occur at a greater distance from the borehole than cuttings and cavings, spalled waste is assumed to have the volume-averaged activity of CH-TRU waste rather than the sampled activities of individual waste streams. RH-TRU waste is isolated from the spallings process and does not contribute to the volume or activity of spalled material.

Further description of this model is provided in U.S. DOE (1996), Appendix PEER 1, Section 3.14.1:

The Spallings conceptual model is one of several that address the calculation of direct waste release to the ground surface if an exploration borehole penetrates a waste panel. Other

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associated models include Cuttings and Cavings, Exploration Boreholes, Repository Fluid Flow, and Multiple Intrusions.

Spallings are the particulate materials introduced into drilling mud by the movement of gas from the waste into the borehole annulus. At one time, spallings were conceived to involve three mechanisms: blowout, stuck pipe, and gas-induced spall. Because the latter two were perceived to produce insignificant releases, DOE determined that this model would concentrate on blowout. The repository pressure domain, where spallings are applicable, is above the borehole fluid hydrostatic pressure because it can occur only when the repository gas pressure is capable of countering and reversing the mud-laden drilling fluid during the drilling process. When the drillhole annulus around the drill pipe is cleared of drilling fluid, it becomes a conduit for free release of repository gases.

The principal parameters in the Spallings model are the gas pressure, the volume of gas in the repository when it is penetrated, and properties of the waste such as particle diameters and resistance to erosion. Because the release associated with spallings 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 (U.S. DOE (1996), Appendix PEER 1, Section 3.14.1).

The CMPR and the U.S. EPA found the original spallings conceptual model to be inadequate, but after the DOE submitted additional information regarding spall analogs, surrogate waste strength, the occurrence of maximum pressure gradients and other factors, the panel determined that the model results were conservative and acceptable for use in the CCA (U.S. DOE, 1997, Section 3.1).

16.2 Changes since the CCA

(Conceptual Model Change) In preparation for the CRA-2004 the U.S. DOE developed a replacement spallings model, which a peer review found to be adequate (U.S. DOE, 2003b, Spallings Conceptual Model Peer Review Report). Results of the peer review were also described in the CRA-2004 (U.S. DOE, 2004, Section 9.3.1.3.5).

The conceptual model for spallings is summarized in the context of the software (DRSPALL) which implements the model (SNL, 2003):

DRSPALL is based on the theory of one-dimensional time-dependent compressible isothermal fluid flow. Somewhat different forms of that theory are used, depending on whether the flow is in the wellbore or in the repository, and whether the wellbore currently penetrates the repository or not. The wellbore and repository flows are coupled at a specified boundary by a set of conditions. Schematic diagrams of the flow geometry prior to and after penetration are shown in Figure 3-1 and Figure 3-2, respectively. Throughout the process, the drill bit can move downward as a function of time, removing salt or waste material. Flow in the well is treated as a compressible, viscous, multi-phase mixture of mud, gas, salt, and possibly waste solids. Flow in the repository is treated as viscous, compressible single-phase gas flow in a porous solid. At the cavity forming the repository-wellbore boundary (following penetration) waste solids freed by drilling, tensile failure, and associated fluidization may enter the wellbore flow stream. Between

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> *the well and the repository, flow is treated according to the state of penetration, as described later* (SNL, 2003, Section 3.0)

Spallings is conceptualized to occur in three stages:

- pre-penetration, before the drill bit intersects the waste panel volume;
- transition, occurring as the drill bit nears the waste panel volume when the repository and wellbore are in hydraulic communication;
- post-penetration, when the drill bit has penetrated the repository.

Further details describing the spallings conceptual model during each stage are found in SNL (2003), Sections 3.1 through 3.6.

17 Direct Brine Release

17.1 Description in the CCA

The direct brine release (DBR) conceptual model is described in U.S. DOE (1996), Section 6.4.7.1.1:

> *Direct brine release refers to the possibility that brine containing actinides may flow from the waste panels up a borehole to the surface during drilling (Appendix MASS, Section MASS.16.2). It is conceptualized that direct brine release to the surface will not occur every time a borehole penetrates the waste panels but rather that it can occur only when two conditions are met. The first condition is the presence of mobile brine in the waste panels. Because of brine consumption by corrosion and low initial saturation, it is possible for liquid saturations below the residual saturation to exist in the repository, in which case direct brine release cannot occur. The second condition is the pressure in the waste panels must be greater than the pressure at the base of the column of drilling mud. Drillers in the Delaware Basin use a salt-saturated mud with a specific gravity of about 1.23 while drilling through the Salado. This corresponds to a pressure of approximately 8 megapascals at the repository horizon (see Appendix MASS, Section MASS.16.2, and MASS Attachment 16-2). If fluid in the waste panels is below this pressure, no direct brine release during drilling can occur because liquid flow in the repository will be away from the borehole.*
>
> *In the conceptual model, resolution of the details of flow near the borehole is considered important, as the changing physical conditions over the short duration of this flow can significantly impact estimates of the total volume released. It is not assumed that a direct brine release would be noticed by the driller (EPA 1996a, 61 FR 5230). Also important to the conceptual model is how long direct brine release occurs. There are several ways in which the direct brine release could be stopped. A driller might detect higher flow rate to the mud pit and take action to mitigate consequences. Alternatively, direct brine release will stop when the driller cases the hole after reaching the base of the salt section. As discussed in Appendix MASS (MASS Attachment 16-2) and Appendix DEL (Section 7.5), the DOE assumes that for low volumes of fluid flow, the borehole will be controlled and cased within 72 hours after the penetration of the*

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repository. In all cases, all fluid flow to the surface during drilling is assumed to cease within 11 days after penetration of the repository.

In the conceptual model for direct brine release, several other assumptions are made that relate to other conceptual models. The processes of direct solids release from cuttings, cavings, spall, and direct brine release are treated separately, although the direct brine release model does account for the effects of solids removal (spall) on fluid flow near the well bore. Direct brine release will affect the pressure and saturation in the repository. However, it is assumed that these effects are negligible over the long-term because of their transient and local nature, and they are not accounted for in long-term (10,000-year) BRAGFLO disposal system calculations. This assumption simplifies modeling because it allows detailed consideration of direct brine release over a short time period, without having to couple the results of these calculations back into the disposal system simulations.

The area over which fluid flow can occur during direct brine release is assumed to be the rooms and drifts of waste panels, the DRZ, room pillars, and panel closures. Because local scale, short-duration flow is important, the geometry of the waste panels is considered important and is represented in the model. It is assumed that the flow interactions with the Salado other than the DRZ are not important during direct brine release. For this model, pillars are arbitrarily assumed to have the properties of the DRZ rather than intact halite, although in reality their properties are probably like a DRZ at their edge and like intact halite in their core. Since the DRZ permeability is greater than the permeability of intact halite, this assumption is conservative. A two-dimensional geometry is used parallel to the repository horizon, with a 1° dip from north to south.

17.2 Changes since the CCA

(Conceptual Model Change)[5] In 2021, the CCMPR considered changes to DBR conceptual model. Specifically, the envisioned additional waste panels, lying to the west of the current operations area, introduce excavated regions that were not previously considered in the DBR conceptual model or its implementation in a computational grid (Falta et al., 2021, Section 3.0). The mathematical model that implements the direct brine release conceptual model is not affected by the new excavated regions (Hansen, 2021). The peer review found the DBR conceptual model to be adequate and reasonable after the changes introduced to represent the additional waste panels (Falta et al., 2021, Section 4.3).

18 Castile and Brine Reservoir

18.1 Description in the CCA

The conceptual model for the Castile and for brine reservoirs in the Castile is described in U.S. DOE (1996), Section 6.4.8:

For performance assessment, the Castile is conceptualized as unimportant because of its expected low permeability (based on similarities to the Salado), unless a borehole penetrates

[5] These changes are currently pending approval of RPPCR by the EPA.

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> *both the repository and a brine reservoir in the Castile. Two regions are specified in the Castile horizon in the disposal system geometry: the Castile (Region 29 in Figure 6-13) and a reservoir (Region 30 in Figure 6-13). The Castile region is assigned an extremely low permeability, which prevents it from participating in fluid flow processes, consistent with the concept that it is unimportant*.
>
> *Where they exist, Castile brine reservoirs in the northern Delaware Basin are believed to be fractured systems, with high-angle fractures spaced widely enough that a borehole can penetrate through a volume of rock containing a brine reservoir without intersecting any fractures and therefore not produce brine. They occur in the upper portion of the Castile (Popielak et al. 1983, G-2). Appreciable volumes of brine have been produced from several reservoirs in the Delaware Basin, but there is little direct information on the areal extent of the reservoirs or the interconnection between them. The WIPP-12 data indicate that fractures in the network have a variety of apertures and permeabilities, and they deplete at different rates. Brine occurrences in the Castile behave as reservoirs—that is, they are bounded systems—rather than as aquifers such as groundwater in the Culebra and Magenta. The properties that need to be specified for brine reservoirs are pressure, permeability, compressibility, total brine volume, and porosity.*

In its review of the CCA, the U.S. EPA found that "DOE's discussion of the size, orientation, and repressurization potential of the Castile brine reservoirs was not well supported" (U.S EPA, 1998b, page 14-30). As a result, the U.S. EPA required the U.S. DOE to conduct an analysis termed the PA Verification Test (PAVT) (U.S. EPA, 1998c) that used different parameters to describe the occurrence and hydraulic properties of the Castile brine reservoirs (U.S. EPA, 1998a). In light of that analysis, the U.S. EPA "found that the original brine reservoir characteristics were, in fact, acceptable." (U.S. EPA, 1998b, page 14-31).

18.2 Changes since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

19 Multiple Intrusions

19.1 Description in the CCA

The conceptual model for multiple intrusions is described in several sections of U.S. DOE (1996), Appendix PEER 1, Section 3.17.1:

> *The Multiple Intrusion conceptual model is an extension of the Exploration Borehole model that describes fluid flow between the repository and multiple exploratory boreholes penetrating a single waste panel. The borehole drilling methods and frequencies, borehole plugging, and plug degradation discussed in the Exploration Borehole model in Section 3.12 are the same for multiple intrusion boreholes. Short-term flow through unsealed boreholes is addressed in the Direct Brine Release conceptual model in Section 3.15* (U.S. DOE, 1996, Appendix PEER 1, Section 3.17.1).

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U.S. DOE (1996) Section 6.3.2.2 describes the Disturbed Performance Deep Drilling Scenario that conceptualizes the effect on the repository and releases to the accessible environment resulting from a future drilling intrusion. The Exploration Borehole conceptual model describes the features and properties of an intrusion borehole.

The occurrence of future drilling intrusions is conceptualized as a stochastic process with a constant drilling rate:

> *Drilling events are assumed to be random in time and space* (U.S. DOE, 1996, Section 6.4.12.3).

Drilling intrusion events are categorized as E1 or E2:

> *The DOE has distinguished two types of deep drilling events by whether or not the borehole intersects a Castile brine reservoir. A borehole that intersects a waste disposal panel and penetrates a Castile brine reservoir has been designated an E1 event. […] A borehole that intersects a waste panel but does not penetrate a Castile brine reservoir has been designated an E2 event* (U.S. DOE, 1996, Section 6.3.2.2).

The effects of intrusions on the repository and the resulting releases are modeled by three disturbed performance scenarios (U.S. DOE, 1996, Section 6.3.2.2):

- The E1 scenario, in which one drilling intrusion of type E1 occurs in a waste panel.
- The E2 scenario, in which one or more drilling intrusions of type E2 occurs in a waste panel.
- The E1E2 scenario, in which any number of drilling intrusion occur in the same waste panel and at least one intrusion is of type E1.

Individual intrusions are classified as either E1 or E2, depending on whether the intrusion penetrates a Castile brine reservoir. When multiple intrusions occur in the same waste panel, the Multiple intrusions conceptual model describes how flow and transport results are determined. The Multiple intrusions conceptual model relates any sequence of intrusions to one of the three disturbed performance scenarios.

Table 2. Summary of multiple intrusion scenarios

Sequence of First Two Boreholes	Basis for Brine Flux and Radionuclide Transport
E2 followed by E1	E2 scenario until the time of the second intrusion, thereafter E1E2 scenario
E1 followed by E2	E1 scenario until the time of the second intrusion, thereafter E1E2 scenario
E1 followed by E1	E1 scenario until the time of the second intrusion, thereafter E1E2 scenario
E2 followed by E2	E2 scenario

Adapted from U.S. DOE (1996), Appendix PEER 1, Table 3.17.1.

In the case of a third or subsequence drilling intrusion, the rules in the above table are applied. To summarize, effects and releases from any sequence of only E2 intrusions are conceptually modeled by the effect and releases calculated for the E2 scenario, because:

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> *In cases of two E2 penetrations, long-term brine release volume is assumed to be the same as for a single E2 penetration because flow will be controlled by the rate at which brine can be supplied by the Salado halites, rather than the rate at which brine can flow in the borehole* (U.S. DOE, 1996, Appendix PEER 1, Section 3.17.1).

Effects and releases from any sequence including one or more E1 intrusions are modeled by:

- the results of the scenario corresponding to the type of the first intrusion until the time of the first E1 intrusion following the initial intrusion.
- the results of the E1E2 scenario after each additional E1 intrusion until the time of the following E1 intrusion.

19.2 Changes Since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

20 Climate Change

20.1 Description in the CCA

The climate change conceptual model is described in U.S. DOE (1996), Section 6.4.9:

> *The present climate at the WIPP and the geologic record of past climate change in southeastern New Mexico are discussed in Section 2.5 and Appendix CLI. Although meaningful quantitative predictions of future climate for the next 10,000 years are not feasible for the WIPP (or any location), effects of reasonably possible climate changes on disposal system performance must be considered. For the WIPP, uncertainty about these effects is incorporated in the performance assessment by considering the effects of various possible future climates on groundwater flow and potential radionuclide transport in groundwater. Direct effects of climate change that do not involve groundwater flow do not affect the long-term performance of the WIPP because of its depth below the land surface. Examples of such direct effects are changes in wind patterns, thermal effects related to changes in surface temperature, and near-future impacts on surface facilities. Long-term effects of climate change on the near-surface portions of the shaft seal system (see Section 6.4.4) are not incorporated in the analysis because BRAGFLO modeling conducted for this performance assessment indicates that system performance is unaffected by the behavior of the upper portion of the shaft seal system. Additional aspects of climate change screened out from the performance assessment, including glaciation at the site and possible future anthropogenic changes, are discussed in Appendix SCR (Sections SCR.1.6.2 and SCR.3.6.1).*
>
> *The effects of postulated climate change on groundwater flow have been evaluated outside of the performance assessment calculations using a regional three-dimensional groundwater basin model based on the concept of basin hydrology introduced in Section 2.2.1.1. For the purposes of the regional analysis, climate-related factors that might affect groundwater flow, such as precipitation, temperature, and evapotranspiration, are treated through a single model parameter, potential recharge, which controls the rate at which water is added to the model at the water table. As described in Appendix MASS (Section MASS.17 and MASS Attachment 17-1),*

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changes in this parameter allow simulation of regional groundwater flow under a range of different future states in which the climate may be wetter, the water table may be higher, and groundwater velocity in all units may increase. These and other simulations discussed in Appendix MASS (Section MASS.15 and MASS Attachment 15-7), show that the regional, three-dimensional effects of climate change can be reasonably approximated in performance assessment through direct scaling of specific discharge in the two-dimensional, steady-state groundwater velocity field for the Culebra.

20.2 Changes since the CCA

This conceptual model is unchanged since the 1996 CCA.

21 Creep Closure

21.1 Description in the CCA

The creep closure conceptual model is described in U.S. DOE (1996), Section 6.4.3.1:

Salt creep occurs naturally in the Salado halite in response to deviatoric stress. Inward creep of rock and the repository response is a process generally referred to as creep closure. Creep closure of excavated regions begins immediately because of excavation-induced deviatoric stress. If the rooms were empty, closure would proceed to the point where the void volume created by the excavation would be eliminated as the surrounding formation returns to a uniform stress state. In the waste disposal region, waste consolidation will continue until loading in the surrounding rock is uniform, at which point salt creep ceases. The amount of waste consolidation that occurs and the time it takes to consolidate are governed by properties of the waste (waste strength, modulus, etc.), properties of the surrounding rock, the dimensions and location of the room, and the quantities of fluids present in the room (U.S. DOE, 1996, Section 6.4.3.1)

Closure of the repository occurs naturally in the Salado halite as a response to the imbalance of forces created by excavation of the repository rooms and passages. Weak and plastic rock salt begins immediately to flow into the excavated spaces by processes dominated by creep. The rate of closure is the combined result of creep rates inherent to salt, repository temperatures and pressures, and resistance provided by repository contents. The creep rate proceeds to the limits determined by resistance from gas, brine, waste, backfill, or other contents in the repository until the void space is closed to the final porosity dictated by waste and seal material properties, contained fluid pressure, and lithostatic pressure. Roof fall in the disposal rooms, which may have significant impact on flow at least in the short term, is not included in the model.

Both brine and gas content of the repository vary with time. Brine inflow/outflow is partly controlled by gas pressures. The relationship between gas outflow rates and gas generation rates influences pressures within the repository. Gas pressure results from the alteration of waste by biogenic and corrosion-based processes. The rate of the corrosion process is dependent on brine availability. Repository gas and brine pressures are limited by the minimum pressures at which gas or brine would be forced out of the repository via identified flowpaths through fractured interbeds within the Salado. The threshold pressures for initiation of outflow through

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these fractured anhydrite interbeds are therefore a key consideration in limiting resistance to closure due to gas and brine pressures. The fractures in the interbeds are essentially horizontal, so the pressures necessary to open the fractures or to initiate new fractures must be greater than the lithostatic load. Further, some resistance to gas release may result from travel through the fractured, rock-bolted halite between the repository and the interbeds. Resistance to gas outflow due to stress cage effects at the repository boundary and gas pressures necessary to maintain very extensive fractures may result in repository pressures larger than interbed threshold pressures. Gas pressures, which are some amount greater than the lithostatic pressure, are therefore possible at some times during the repository gas generation history. Internal gas pressures greater than the stress imbalance that drives creep inflow are conceivable. Internal pressures may contravene stresses in the salt and repository closure may cease, or repository inflation may occur in some scenarios. The stoichiometric treatment of time histories of gas generation and the volumetric model based on creep closure rates and waste compaction are combined in the SANTOS computer code to provide repository void volume estimates through time as part of lookup tables called the "porosity surface." (U.S. DOE, 1996, Appendix PEER 1, Section 3.19.1).

21.2 Changes since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

22 Shaft and Shaft Seals

22.1 Description in the CCA

The conceptual model for the shaft and shaft seals is described in U.S. DOE (1996), Section 6.4.4:

The four shafts connecting the repository to the surface are represented in performance assessment with a single shaft, represented by Regions 2 through 11 on Figures 6-13 and 6-14. This single shaft has a cross section and volume equal to the total cross section and volume of the four real shafts it represents and is separated from the waste disposal regions in the model by the true north-south distance from the waste to the nearest shaft (the Waste Shaft). Upon closure of the repository, the shafts will be sealed as described in Section 3.3.1. The seal system is represented in performance assessment by discretizing 11 model regions in the shaft. These regions are as follows: an earthen fill region above the Rustler; a compacted clay column in the Rustler; an asphalt region at the top of the Salado; three concrete sections within the Salado; an upper Salado compacted clay column; a thick section of compacted crushed salt; a lower Salado compacted clay column separated into upper and lower segments; and a concrete monolith at the repository horizon (see Appendix SEAL, Section 4 and Appendix A). The concrete components in the Salado represent the concrete asphalt waterstops in the seal system design. Seal material parameter values used in the performance assessment are provided in Table 6-13.

Conceptually, the shafts are assumed to be surrounded by a DRZ in the Salado. Within the bedded halite, the DRZ begins to form immediately after excavation and develops progressively as a function of unloading as the formation creeps toward the excavated area. From a sealing

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perspective, the most important characteristic of the DRZ is the higher permeability that results from dilatant deformation and the increased pore volume.

The properties of the DRZ are known to vary with the type of adjacent material, time, and depth. When the shaft seals are emplaced, back pressures will progressively develop over time as the surrounding salt creeps inward. The back pressure applied by the seal material will progressively reduce the magnitude of the stress differential, which is the source for the DRZ microfracturing mechanism. The back pressure also results in a higher mean stress, which induces healing of the DRZ. The shaft DRZ permeability will, over time, approach that of the intact halite. Also, since the creep rate of the salt surrounding the shafts depends on depth, the back pressures supplied by the seal materials will result in DRZ healing at rates that increase with depth. The relative stiffness of the seal material is a factor, as well.

In the performance assessment model, the radial extent of the DRZ around the shaft seal materials is an input parameter obtained by numerical model calculations and is corroborated by field data (see Appendix SEAL, Section 8 and SEAL Appendix C). The permeability of the DRZ around the shaft versus distance is assumed to follow a log linear relationship. Permeability of the DRZ at the shaft wall is based on experimental data collected in the air intake shaft (Dale and Hurtado 1996) and Room M (Van Pelt 1995). More information on how the DRZ is incorporated into the shaft parameters is contained in Appendix PAR (Parameter 12).

The DRZ surrounding the shaft is not represented explicitly in the BRAGFLO mesh (Figures 6-13 to 6-15). Rather, the mesh has been simplified to represent only the cross-sectional area of the four WIPP shafts, and the permeability values for the various seal components at different times have been adjusted to account for the presence of the shaft DRZ. This adjustment, which yields effective permeabilities, can be done because in Darcy flow the flux through a porous medium is a linear function of the product of the permeability of the medium and the cross-sectional area across which flow occurs. Thus, the flux that would occur through a shaft and its surrounding DRZ can be modeled equivalently using the shaft cross-sectional area with a higher seal component permeability. Equations for the derivation of the effective permeabilities are given in Appendix PAR (Parameter 12) and Appendix IRES (Section IRES.2) (U.S. DOE, 1996, Section 6.4.4).

22.2 Changes since the CCA

(Conceptual Model Change) In the CCA, the shaft seal system was represented by 11 discrete model regions each with different material properties and a sequence of time-dependent material property changes. In 2003, prior to the CRA-2004, the shaft seal system representation was replaced with a simplified, two-layer system with fewer time-dependent changes that maintains permeability equivalent to the original 11-layer system (U.S. DOE, 2004, Section 6.4.4). The Salado Flow Peer Review concurred that the simplified shaft model "conservatively represents the behavior of seal components and is valid." [U.S. DOE, 2004, Appendix PEER 1, Section 2.1.2 (see Section 3.1.2.2 therein)] The simplified shaft seal model has been used in WIPP PA from the CRA-2004 to present.

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23 Gas Generation

23.1 Description in the CCA

The original gas generation conceptual model is described in U.S. DOE (1996), Section 6.4.3.3:

> *Gas will be produced in the repository because of a variety of chemical reactions, primarily those occurring between brine, metals, microbes, cellulosics and similar materials, plastics, and rubber materials, and via liberation of dissolved gases to the gas phase. The dominant processes are anoxic corrosion of metals in the waste containers and the waste and microbial degradation of cellulosics, plastics, and rubbers in the waste. Anoxic corrosion reactions will occur between brine and steel, aluminum, and aluminum alloys, producing H_2. Microbial degradation of cellulosics may produce a variety of gases; however, for the waste inventory and expected conditions, CO_2 and CH_4 (methane) are expected to be the dominant gases for the process. Radiolysis has been demonstrated by laboratory experiment and model calculations to be insignificant (see Appendix MASS, Section MASS.8; Appendix SCR, Section SCR.2.5.1.3).*
>
> *Performance assessment uses the average stoichiometry model to estimate gas generation occurring in the waste disposal region. […] The average stoichiometry model accounts for the formation of gas by anoxic corrosion of steels and microbial degradation of cellulosics, including plastics and rubbers. For the purpose of calculating repository pressure and gas flow, the density and viscosity of the generated gas are assumed to be those of H_2. In the average stoichiometry model, gas is assumed to be generated at a rate dependent on the availability of brine in the computational cell. Gas can be generated by anoxic corrosion in all realizations, and is assumed to be generated by microbial degradation in half of the realizations. The average stoichiometry model is based on experimental data on the rates of corrosion and microbial degradation under inundated and humid conditions. These data were used to develop ranges of possible gas-generation rates, as shown in Table 6-10. In BRAGFLO, a gas-generation rate is determined from the rates listed in Table 6-10 by a linear interpolation method that combines humid and inundated rates based on the effective liquid saturation (Appendix BRAGFLO, Section 4.13). The effective liquid saturation in a computational cell in BRAGFLO for the purpose of gas generation is the computed liquid saturation in that cell, plus an adjustment to account for uncertainty in the capillary rise (wicking) characteristics of the waste. Refer to Appendices PAR (Parameter 8) and BRAGFLO (Sections 4.13 and 7.2.9) for details on the treatment of wicking in the gas generation model.*
>
> *Anoxic corrosion is represented by a generic equation given in Appendix BRAGFLO (Section 4.13). This equation accounts for corrosion only of the steel content in the repository by the reaction expected to dominate. Because the total quantity of aluminum and aluminum alloys is a small compared to the quantity of iron base metals, corrosion of aluminum is omitted for simplicity. The steel content of the repository is depleted separately in each computational cell (that is, a cell-by-cell basis), and gas generation can continue in cells, depending on parameter values, until all steel in a cell is consumed. Brine in cells is consumed as gas generation proceeds. If a cell has a brine saturation equal to zero, it cannot produce gas by anoxic corrosion.*

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It is assumed that there is no passivation of anoxic corrosion of steel by CO_2 and H_2S produced by microbial degradation because microbial gas generation is too slow and also because CO_2 will be removed from the gaseous phase by reaction with MgO backfill.

Microbial degradation occurs in only half of the realizations because of uncertainties in viability of the microbial colonies (Appendix MASS, Section MASS.8 and MASS Attachment 8-2). Like anoxic corrosion, microbial degradation is represented by a generic equation, given along with other details in Appendix BRAGFLO (Section 4.13). […] It is assumed that the microbial degradation process neither produces nor consumes water, but its rate is dependent on the amount of liquid present in a computational cell.

Microbial degradation may consume plastic and rubber materials in the repository. The DOE assumes that in half of those simulations in which microbial degradation of cellulosics occurs, microbial degradation also acts on plastic and rubber materials in the waste disposal region.

23.2 Changes since the CCA

The gas generation conceptual model has changed in one aspect since the 1996 CCA. The original gas generation conceptual model acknowledges that gas may be generated by a variety of processes and includes and describes those processes which are dominant contributors to gas in the repository. In the FEP screening process, the CCA excluded FEPs related to radiolytic gas generation on the basis of low consequence: "*Radiolysis has been demonstrated by laboratory experiment and model calculations to be insignificant"* (CCA, Appendix MASS, Section MASS.8; Appendix SCR, Section SCR.2.5.1.3). For the CRA-2019, changes in the waste inventory prompted a re-evaluation of the potential contribution to gas generation due to radiolysis. This re-evaluation determined that radiolysis of brine has the potential to be "a significant gas generation source" (Day, 2019). A model for radiolysis of brine was formulated as described below. Gas generation by radiolysis of other materials, notably CPR, was determined to not have "a significant impact on the performance of the repository" (Day, 2019), and related FEPs remain excluded.

Radiolysis of brine in the WIPP repository produces only H_2 gas. Other radiolytic products, e.g., hydroxide, are not modeled. The rate of H_2 production can be modeled using a G-value, i.e., a count of molecules of H_2 generated per 100eV of energy absorbed in brine. Radiolytic energy is deposited in brine by alpha particles emitted from dissolved and wetted-solid radionuclides. Gamma radiation is not considered due to 1) low gamma radiation in the WIPP waste inventory and 2) lower G values for gamma radiolysis of water than from alpha radiolysis. Not all wetted-solid radionuclides contribute to radiolytic gas generation because alpha particle disintegration energy can be attenuated in the particles containing the radionuclides.

24 Chemical Conditions

24.1 Description in the CCA

The chemical conditions conceptual model is best described in U.S. DOE (1996), Appendix PEER 1, Section 3.22.1:

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The chemical conditions of the repository are a major influence on actinide solubility. It has been estimated that under specific chemical conditions (low pH), the actinide solubility may increase over expected values by up to five orders of magnitude. This model has used engineering systems to limit such variability. DOE has assumed that equilibrium has been established between the brine in the repository (Castile or Salado), waste forms, and primary minerals. In addition to this basic chemical assumption, a series of other assumptions were made to help facilitate computer code calculations. The assumptions are discussed in further detail below. The defense of model assumptions is presented in Appendix SOTERM, which was not available for the peer review.

Major variables in this conceptual model include brine compositions (fixed chemistry Salado and Castile brines), ligand concentrations, pH, fCO_2, oxidation conditions, mineral stabilities, cement inventories, actinide inventories, and MgO backfill. Of these variables, some can be held constant because of the MgO backfill. The reaction of MgO and CO_2 acts to buffer the pH of the repository and allows other variables to be fixed. The two major variables that will now be constrained are fCO_2 (low fugacity) and pH (between 9 and 10, depending on brine composition).

Certain assumptions are critical to this model. Brine and waste are modeled as a uniform mix of dissolved and solid phases. Thermodynamic equilibrium is assumed for dissolved actinides but not for redox reactions amongst the actinides. Further, chemical homogeneity and solubility equilibrium are assumed. This allows for the assumption of instantaneous reactions. Chemical microenvironments are not believed to persist for this reason. DOE assumes there will not be conditions whereby supersaturation can exist for long periods of time. Temperatures will increase a total of approximately 5.4°C (radioactive decay and exothermic reactions), and it is assumed that there will be negligible effects due to this increase.

DOE believes that calculating mixing of brine from different sources is not amenable to performance assessment. Therefore, brine compositions are fixed by performance scenarios. Undisturbed performance and E2 scenarios dictate the use of Salado brine. This is because the Castile Formation is not penetrated. Scenarios E1 and E1-E2 use Castile brine as the solvent for chemical conditions.

Oxidation states of the repository are believed to be reduced. This judgment is based on the thought that available oxygen will be consumed early by oxic corrosion or aerobic microbes. Furthermore, large quantities of iron from 55-gallon drums are consumed by anoxic corrosion, producing hydrogen gas and ferrous iron. Although reducing conditions are expected, redox reactions between dissolved actinides in possible oxidation states are not addressed. DOE assumes this will produce conservative results and increase the total dissolved actinide source term.

Experimental data have shown that acidic conditions greatly enhance the solubility of actinides. Although cement materials in the waste will hydrate to $Ca(OH)_2$, CO_2 produced by microbial degradation of cellulosics will overwhelm this component and force the brine to low pH values. To reduce the potential for highly accelerated actinide dissolution, DOE decided to add MgO to the repository as backfill. The simplified reactions of concern are:

$$MgO + H_2O = Mg(OH)_2$$

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$Mg(OH)_2 + CO_2 = MgCO_3 + H_2O$

In large enough quantities, the backfill will act as a getter of CO_2 and thereby buffer the liquid, produce low CO_2 fugacities, and provide alkaline conditions in the repository.

Because the addition of MgO will buffer the CO_2 fugacity, many processes that create time-dependent changes in the repository have been negated. The other assumptions imparted on the chemical conditions model, such as fixed ligand inventory, mineral equilibrium (halite, anhydrite, brucite), fixed brine compositions, and fixed actinide inventories have produced a fairly simple system. There is no need for a large computer code to replicate the conditions of the repository. Rather, fixed or calculated (EQ3/6) parameters (pH, fCO_2, phase equilibria, buffering equilibria) from this model are used as input to other, more complex conceptual models (U.S. DOE, 1996, Appendix PEER 1 Section 3.22.1).

The major assumptions of the Chemical Conditions conceptual model have been listed in the model description above. To summarize, the assumptions are as follows:

1. *Brine and waste are modeled as a uniform mix of dissolved and solid phases.*
2. *Thermodynamic equilibrium is assumed for dissolved actinides but not for redox reactions among the actinides.*
3. *Chemical homogeneity and solubility equilibrium are assumed. This allows for the assumption of instantaneous reactions.*
4. *DOE assumes there will not be conditions whereby supersaturation can exist for long periods of time.*
5. *It is assumed that there will be negligible effects due to the temperature increase (by radioactive decay and exothermic reactions) of approximately 5.4°C.*
6. *Brine compositions are fixed by performance scenarios.*
7. *Oxidation states of the repository are assumed to be reduced.*
8. *All CO_2 will be fixed by available $Mg(OH)_2$, thereby buffering the pH of the repository.*
9. *Actinide and ligand inventories are fixed.*

This conceptual model, as described above, was determined to be inadequate by the first and second Conceptual Models Peer Review. The peer panel convened a third time and based on additional information provided by the DOE, the Chemical Conditions conceptual model was found to be adequate (U.S. DOE, 1997).

24.2 Changes since the CCA

(EPA-Mandated Conceptual Model Change) In their review of the 2004 Compliance Recertification Application, EPA "…observed that abundant sulfate was potentially available for sulfate reduction […] because of the presence of anhydrite (CaSO4) in the Salado Formation surrounding the repository." As a consequence, EPA stated that, for modeling of gas generation from microbial degradation of CPR, abundant sulfate should be assumed (U.S. EPA, 2006). In response to EPA's review, the U.S. DOE

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modified the Chemical Conditions conceptual model to reflect an assumption that anhydrite beds act as an unlimited source for sulfate for processes in the repository, specifically for microbial degradation of CPR, both before and after brine inundation. The implementation of the Chemical Conditions model was updated accordingly for the CRA-2004 PABC (Leigh et al., 2005, Section 2.4).

25 Dissolved Actinide Source Term

25.1 Description in the CCA

The dissolved actinide source term conceptual model is described in U.S. DOE (1996), Section 6.4.3.5:

> *Actinides may be mobilized either by dissolution in brine as aqueous species, by bioaccumulation or sorption onto colloidal particles, or by condensation into colloidal forms as actinide-intrinsic colloids that could be carried by brine (see Section 6.4.3.6 for a discussion of colloidal actinides). The dissolved actinide source term model calculates the dissolved concentration of each actinide in solution by applying the modeled solubility for the particular oxidation state, as determined by the oxidation state distribution for that actinide, at the repository conditions presented in Section 6.4.3.4. Several oxidation states are not stable in the chemically reducing conditions described in Section 6.4.3.4. The unstable oxidation states are Np(VI), Pu(V), Pu(VI), and Am(V), as described in Appendix SOTERM (Section SOTERM.4).*
>
> *Thorium will exist only in the IV oxidation state (see Appendix SOTERM, Section SOTERM.4.1). Am and Cm will exist in only the III oxidation state (see Appendix SOTERM, Sections SOTERM.4.4 and SOTERM.4.5). For the remaining actinides, Pu, U, and Np, it is uncertain whether repository conditions will favor the lower or higher of the remaining oxidation states (see Appendix SOTERM, Sections SOTERM.4.2, SOTERM.4.3, and SOTERM.4.6). The DOE has captured the range of possible behavior by assuming that in half the realizations, conditions within the repository are extremely reducing and the solubility of all three of these actinides will be adequately represented by the solubility of their lower oxidation states. In the other half of the realizations, the solubilities of these actinides are well represented by the solubilities of the higher of the possible oxidation states. The factors controlling the aqueous actinide concentration in a possible oxidation state are equilibrium with anhydrite, halite, MgO, and brine.* [U.S. DOE, 1996, Section 6.4.3.5]

U.S. DOE (1996), Appendix PEER 1, Section 3.23.1 provides additional detail on this conceptual model:

> *Several oxidation states can be screened out or substantially constrained. Oxidation states initially screened out are Np (+6), Pu (+5), Pu (+6), and Am (+5). The screening rationale are described in Appendix SOTERM (not provided to the Panel for review). Actinides limited to a single oxidation state are Th (+4), Am (+3), and Cm (+3). The model then assumes that the remaining three actinides will exist in only one oxidation state, but is unsure which of two possible states it will be. Therefore, the modeling assumes half the realizations will be in the reduced state (U+4, Np+4, and Pu+3) and half in the more oxidized state (U+6, Np+5, and Pu+4).*

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The factors controlling dissolved actinide concentrations are equilibrium with anhydrite, halite, MgO, actinide-bearing solid phases, appropriate brine, and water-soluble ligands.

The ligand concentrations used in the calculations are based on the Baseline Inventory Report and are reported to be acetate, citrate, oxalate and EDTA. The concentrations used represent dissolution of the entire ligand inventory. DOE believes this is a conservative approximation for the following two reasons: (1) it does not reduce the ligand inventory by destruction mechanisms, and (2) although all ligands will dissolve in the first brine volume, the ligand concentration will stay constant for the full simulation.

Folded within the dissolved actinide conceptual model are several conceptual submodels. The solubility submodel is the Fracture-Matrix-Transport (FMT) [Note: FMT has been replaced with EQ 3/6] *model, which is based on the Pitzer activity coefficient model of the thermodynamics of highly concentrated electrolytes. This model uses an adaptation of the Harvie-Moller-Weare/Felmy-Weare (HMW/FW) data base. FMT parameters are fitted using the code NONLIN, which calculates the Pitzer parameters. No redox equations are used in FMT; instead, an oxidation state analogy and oxidation distribution state submodel are used.*

Soluble actinide concentrations are based on solubility limits (maximum concentrations), or when a cell is partially depleted, by inventory limits. The actinide inventory is depleted on a cell-by-cell basis for the undisturbed, E1, and E2 scenarios. Processes affecting dissolved actinide concentrations in a computational cell are: dissolution of actinide solids, advection of dissolved actinides by brine flow from neighboring cells, diffusion or dispersion from neighboring cells. And interaction with colloidal particles. The E1-E2 scenario assumes homogeneous mixing within the panel for dissolved actinides moving up the borehole.

As mentioned above, the dissolved actinide source term model incorporates a very critical assumption, that of oxidation state analogy. It assumes that all actinides in the same oxidation state (ex. +III) will form the same aqueous species and isostructural solid phases. There is said to be a large data set confirming this for the 3+ oxidation state, but fewer data exist for the 5+ and 6+ oxidation states. It is also noted that such an analogy may not hold to be strictly true for the 4+ oxidation state. The rationale for using the oxidation state analogy is to allow a great reduction in the number of experiments that must be conducted.

A second assumption is that actinide precipitates formed in laboratory experiments will allow the crystallinity to mature with time. Since solids are typically less soluble than amorphous precipitates, laboratory solubility studies can then provide an upper concentration limit. The exception may be that radiolysis could cause certain solids to become more soluble.

A third assumption in the dissolved species model is that no adsorption will occur with immobile substrates in the disposal rooms. DOE however may take credit for adsorption of dissolved actinides to mineral phases in the Culebra Formation, via the Transport of Dissolved Actinides in the Culebra model.

A fourth assumption considers that dissolved actinide concentrations are also coupled to brine compositions in the disposal rooms. DOE expects this capability to greatly enhance their ability to

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look at site-specific solubilities based on disposal room brines and the effect of engineering modifications on dissolved actinide concentrations.

A fifth assumption centers on the presence of anoxic conditions in the repository setting. Actinide oxidation state distributions are presently unknown, since redox couples are not in equilibrium in low temperature systems. Although it is believed reasonable to expect the actinides to exist in their most reduced state because of anoxic conditions, alpha radiolysis oxidizes Am (III) to Am (V), and Pu (VI) is stabilized in the presence of carbonate. Another potential problem with the assumption is that the repository is actually under oxic conditions for the first few tens of years, due to relict atmosphere and nitrate reactions, and oxidized actinides may encounter kinetic effect problems in attaining their final reduced oxidation state.

25.2 Changes Since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

26 Colloidal Actinide Source Term

26.1 Description in the CCA

The colloidal actinide source term conceptual model is described in U.S. DOE (1996), Section 6.4.3.6:

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

Four types of colloidal particles are believed to cover the range of possible behavior of all colloid types (see Appendix SOTERM, Section SOTERM.6.1.2). The four particle types considered in performance assessment are microbes, humic and fulvic acids (humic substances), actinide-intrinsic (intrinsic), and mineral fragments. The concentration of actinides carried by each colloidal particle type depends on many of the same chemical conditions that govern the concentration of dissolved actinides.

Actinide concentration associated with humic substances and microbes are linked to dissolved actinide concentrations through proportionality constants based on experimental results. For humic substances, actinide complexation constants from WIPP-specific experiments or from published literature are coupled with experimentally determined site-binding densities and solubilities of different types of humic substances in WIPP brines. For microbes, actinide uptake was experimentally determined through experiments with WIPP-relevant bacteria cultures. Actinide concentrations associated with mineral fragment-type colloidal particles are estimated based on results from experiments designed to determine mobile concentrations in brines,

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coupled with site-binding densities of mineral substrates. For the Pu(IV)-polymer, actinide concentrations are determined through solubility experiments conducted from over- and undersaturation over a range of pmH values. Intrinsic colloids of other actinides were determined to be of negligible importance and are eliminated from performance assessment calculations. For more discussion on this topic refer to Appendix SOTERM (Section SOTERM.6.3.2.2).

Actinides associated with microbes and humics are related to the concentration of dissolved actinides in the repository through proportionality constants determined from interpretation of WIPP-relevant experiments and the literature (Appendix SOTERM, Sections SOTERM.6.3.3 and SOTERM.6.3.4). The proportionality-constant relationship is not based rigorously on thermodynamic equilibrium but is simply an empirical relationship. The concentration of actinides associated with the Pu(IV)-polymer is a constant value determined from experimental results at the pmH conditions dictated by the presence of MgO backfill. Likewise, the concentration of actinides associated with mineral colloids is also a constant value, not linked to the concentration of dissolved actinides. Actinides associated with humics and microbes represent most of the colloidal actinide source term. Consequently, the colloidal actinide source term is closely related to the dissolved actinide source term. As discussed in Section 6.4.6.2, however, the source terms are considered separately for transport in the Culebra.

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

U.S. DOE (1996), Appendix PEER 1, Section 3.24.1 provides additional detail on this conceptual model:

The Colloidal Actinide Source Term conceptual model describes the concentration of actinides sorbed to or contained in mobile colloidal particles in the disposal rooms and also describes the stable colloids that must be quantified for transport in the Culebra. The actinides addressed with this model are thorium (Th), uranium (U), neptunium (Np), plutonium (Pu), americium (Am), and curium (Cm). Presently, transport of colloids in the Culebra have not been rigorously modeled because of the complexities of coupling hydrogeology, geochemistry, and colloid chemistry. Because of the chemical complexities of the integrated system and high ionic strength brines present, an attempt has been made to characterize the major colloid types believed to be present in the repository.

The four types described are "hard sphere" carrier colloids (mineral fragments), microbes, soft sphere carrier colloids or hydrophilic colloids (humic and fulvic acids), and intrinsic colloids (true colloids). These particles develop from a variety of processes in the repository, including waste degradation, microbial activity, rock decomposition, and chemical condensation. Intrinsic colloids form by condensation of dissolved actinides in the disposal rooms. Mineral fragments and humic substances provide surfaces that dissolved actinides may sorb to. Microbes actively bioaccumulate actinides intracellularly and also act as substrates for surficially extracellular sorption (Francis 1985).

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Four major decisions have been made that greatly simplify this conceptual model. First, DOE has elected to disregard the effects of competition associated with the equilibrium between dissolved actinides and actinides associated with colloidal particles. Therefore, the two source terms are not inexorably linked, resulting in an overestimation of the total concentration of mobile actinides that may leave the repository. Second, in the event that the sum of the concentrations of the dissolved actinide and colloidal actinide source terms for a particular element exceed the inventory limited concentration of that element, then a partitioning scheme is utilized. Instead of basing the partitioning on an equilibrium approach, DOE has decided to use an approach based on conservatism. The concentration of a particular actinide in the inventory is first made available to the most efficient transport mode. If the inventory is not used up, then the next most efficient transport mechanism is filled. This rationale is continued until the inventory is exhausted by assignment to the five groups of transport vehicles (four colloidal and dissolved actinide source terms). Third, thermodynamic equilibrium is achieved by actinide intrinsic and humic colloids. And fourth, DOE has assumed that microbes and mineral fragments are present in constant quantities in the aqueous phase. This allows a steady state quantity on which the actinides can sorb.

Because of the effect of high ionic strength brines on mineral fragment colloids, which collapses the electric double layer surrounding the colloid, Van der Waals forces can cause agglomeration and settling of such colloids. Laboratory experiments using WIPP brines indicate that this settling effect largely negates mineral fragments as an effective transport mechanism. Thus, DOE has conservatively assigned a mineral fragment concentration for each actinide to be 10^{-9} m/L, one order of magnitude higher than the detection limit of the experiments.[6]

Microbes have a large study base at WIPP, primarily to provide data for the gas generation program. This information has also been helpful in the Colloidal Actinide Source Term model. The source term concentrations associated with microbes are based on actinide uptake experimentally determined from experiments with relevant bacteria cultures.

Humic and fulvic acids are of particular concern because of their well known capability to complex metal cations, including actinides. These soft sphere carrier colloids are not affected by high ionic strength brines, so they may be important in the transport of actinides at WIPP. To determine humic substance concentrations, actinide complexation constants from WIPP experiments or from literature are coupled with site binding densities and solubilities of humic substances in WIPP brines.

Intrinsic colloids are well represented by the Pu(IV) polymer. The mechanism of formation of this polymer has not yet been identified; however, it is known to be stable in high concentrations in highly acidic environments. There is some evidence that the polymerization is strongly linked to hydrolysis, and that it produces an amorphous macromolecule that becomes crystalline with time. This polymer is typically on the order of nanometer size range. Hence, it is assumed to act

[6] Note that the cited value of 10^{-9} m/L for the mineral fragment concentration in the quoted text is different from the value of 2.6×10^{-8} m/L used in the CCA (U.S. DOE, 1996, Appendix SOTERM, Table SOTERM-14).

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like a hard sphere carrier colloid. […] Other actinide intrinsic colloids (especially Am) were found to have negligible importance.

26.2 Changes since the CCA

This conceptual model and associated assumptions are unchanged since the 1996 CCA.

27 Summary and Baseline Maintenance

This document describes the current baseline for the 24 WIPP conceptual models. It is intended that this document will serve as the primary reference for the WIPP conceptual models, and will be used when evaluating new scientific information or changes to the WIPP PA system. Therefore, the descriptions presented here should be updated when any of the following activities or actions occur:

1) Planned changes to the WIPP PA are the subject of formal peer review and approval;
2) Regulatory action such as rulemaking or recertification decisions affect the conceptual models;
3) Regulatory compliance-level PA calculations prompt implementation and/or parameter changes; and
4) Changes to FEPs screening decision result in new conceptual models or changes to existing conceptual models.

A records package in the WIPP Records Center titled “WIPP Conceptual Model Baseline” will be established and all subsequent revisions to this document shall reside therein.

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