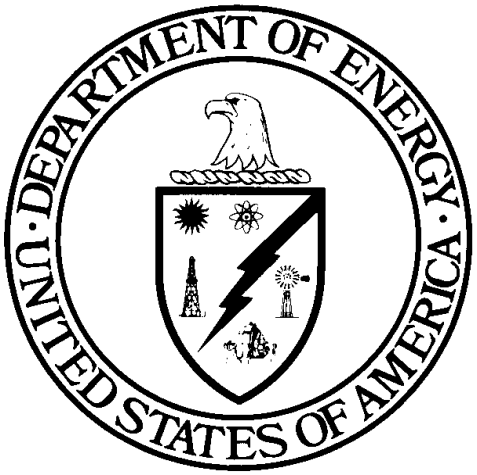
Title 40 CFR Part 191
Subparts B and C
Compliance Recertification
Application
for the
Waste Isolation Pilot Plant

Appendix MASS-2009
Performance Assessment
Modeling Assumptions



United States Department of Energy
Waste Isolation Pilot Plant

Carlsbad Field Office
Carlsbad, New Mexico

Appendix MASS-2009
Performance Assessment
Modeling Assumptions

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Acronyms and Abbreviations

An	actinide
CCA	Compliance Certification Application
CCDF	complementary cumulative distribution function
CH-TRU	contact-handled transuranic
cm	centimeters
CPR	cellulosic, plastic, and rubber
CRA	Compliance Recertification Application
DBR	direct brine release
DOE	U.S. Department of Energy
DRZ	disturbed rock zone
EPA	U.S. Environmental Protection Agency
FEIS	Final Environmental Impact Statement
FEP	feature, event, and process
ft	foot
gal	gallon
in.	inch
INL	Idaho National Laboratory
km	kilometer
LHS	Latin hypercube sample
m	meter
MB	marker bed
MPa	megapascals
NIST	National Institute of Standards and Technology
OS	operating system
PA	performance assessment
PABC	Performance Assessment Baseline Calculation
PAVT	Performance Assessment Verification Test
PR	productivity ratio
QA	quality assurance
RH-TRU	remote-handled transuranic
RoR	rest of repository

SMC	Salado Mass Concrete
SNL	Sandia National Laboratories
T field	transmissivity field
TRU	transuranic
WIPP	Waste Isolation Pilot Plant

Elements and Chemical Compounds

$CaCO_3$	calcite
CH_4	methane
CO_2	carbon dioxide
H_2	hydrogen
H_2O	water
H_2S	hydrogen sulfide
$Mg(OH)_2$	brucite, magnesium hydroxide
$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$	hydromagnesite
MgO	magnesium oxide

MASS-1.0 Introduction

This appendix presents supplementary information to Appendix PA-2009 regarding the assumptions, simplifications, and approximations used in the models of the second recertification performance assessment (PA) of the Waste Isolation Pilot Plant (WIPP) called the 2009 Compliance Recertification Application (CRA-2009) PA. Within this appendix, relevant issues in the formulation or development of the various types of models (for example, conceptual, mathematical, numerical, or computer code) used for the topic under consideration in each section are discussed, and references to relevant historical information are included where appropriate. The CRA-2009 PA is similar to the CRA-2004 PA used in the first recertification of the WIPP. The technical baseline for the first recertification includes the modifications required by the U.S. Environmental Protection Agency (EPA) during their review of the CRA-2004 PA (Cotsworth 2005). These required modifications resulted in a PA called the Performance Assessment Baseline Calculation (PABC), or the CRA-2004 PABC. The CRA-2009 PA is not significantly different than the CRA-2004 PABC. The differences include error corrections, updated parameters, and new software code versions. This appendix references the Compliance Certification Application (CCA) (U.S. Department of Energy 1996) and the CRA-2004 (U.S. Department of Energy 2004) when the information discussed has not changed from past demonstrations of compliance with the EPA's disposal standards. Some of the information important to PA methodology has been repeated from the CRA-2004, Appendix PA, Attachment MASS for completeness.

Section MASS-2.0 contains a summary of changes in PA since the CRA-2004. Section MASS-3.0 includes a discussion of general modeling assumptions applicable to the disposal system as a whole, including a table of assumptions made in PA models, with cross-references. The remainder of this appendix discusses assumptions specific to the conceptual models used in the CRA-2009 PA. Historical development of the WIPP conceptual models that led to the PA used in the CCA is documented in the CCA, Appendix MASS, Section MASS-2.0. Historical development of the modeling assumptions for the CRA-2004 PA is documented in the CRA-2004, Appendix PA, Attachment MASS.

MASS-2.0 Summary of Changes in Performance Assessment

Since the CCA, there have been changes to a number of the conceptual models and processes important in assessing the performance of the WIPP. Changes for the first recertification were discussed in the CRA-2004, Chapter 9.0, Section 9.3.1.3, and Appendix PA, Attachment MASS. Other recertification-related, EPA-mandated changes were documented in the CRA-2004 PABC (Leigh et al. 2005). The technical baseline used to demonstrate continued compliance with the EPA's disposal standards was documented in these two documents. Since this time, ongoing confirmatory experiments, monitoring results, and operational practices have generated information relevant to the features, events, and processes (FEPs), modeling assumptions, and conceptual models for PA, and provided additional support to the conceptual basis of PA. The results of these investigations are included in a new PA for this recertification. Appendix MASS-2009 has been updated to include the impacts of these ongoing investigations and results. Included in the CRA-2009 PA are changes that have occurred since the CRA-2004 PA and new information that is important to PA. These changes are

1. Reassessment of FEPs
2. Compliance monitoring
3. Experimental activities
4. Assessment of model and systems changes and updates
5. Incorporation of CRA-2004 PABC changes, including
    A. Parameter changes: solubility parameters; solubility uncertainty ranges; probability of microbial cellulosic, plastic, and rubber (CPR) degradation
    B. Error corrections
    C. Inventory updates
    D. Changes to CPR degradation implementation
    E. New Culebra transmissivity fields (T fields)
6. Incorporation of CRA-2009 changes, including
    A. The parameter representing the maximum flow duration for direct brine releases (DBRs)
    B. The sampling method applied to the humid and inundated CPR degradation rates
    C. Additional chemistry parameters
    D. Capillary pressure and relative permeability models
    E. Updated drilling rate

F. Parameter corrections – emplacement material parameters, halite/disturbed rock zone (DRZ) porosity, and fraction of the repository occupied by waste

G. Input file corrections

7. Operational considerations

A summary of each change is presented in this section. References to appropriate sections of this appendix are provided for those changes that impact modeling assumptions. In addition, references are provided to other sections of the CRA-2009 where implementation of the changes is discussed.

MASS-2.1 FEPs Assessment

In the WIPP PA methodology (see Appendix PA-2009, Section PA-2.3), FEPs are elements used to develop the conceptual models and modeling assumptions represented in PA. The process used to develop and screen FEPs is outlined in Appendix SCR-2009, Section SCR-2.0. The results of the CRA-2004 FEPs screening are documented in the CRA-2004, Appendix PA, Attachment SCR. For the CRA-2009, a reassessment of the CRA-2004 baseline FEPs was conducted to determine whether changes in WIPP activities and conditions affected the original FEPs descriptions, bases, or screening decisions. This assessment also determined whether additional FEPs should be included in the CRA baseline. The reassessment results are documented in Appendix SCR-2009, Section SCR-3.0 and Section 32 of this application, Scope of Performance Assessment. Changes to the baseline FEPs include updating screening arguments with new information that has become available and separating general FEPs into more descriptive FEPs. No changes to PA implementation or modeling assumptions were made as a result of the FEPs reassessment because no FEPs that were previously screened out of PA calculations have been screened in and no FEPs that were screened in have been screened out.

MASS-2.2 Monitoring

Monitoring activities have continued since the certification of the WIPP. These activities are used to validate assumptions and PA parameters, and to detect substantial and detrimental deviation from expected repository performance. Monitoring, as discussed here, applies to the assurance requirement of 40 CFR § 191.14(b) (U.S. Environmental Protection Agency 1993) and the monitoring criteria at 40 CFR § 194.42 (U.S. Environmental Protection Agency 1996). Appendix MON-2009 details the monitoring program that meets these requirements. The monitoring program was assessed to determine if the results indicate that changes should be made to the monitoring program. The results did not indicate that changes were required (Wagner 2008). The monitoring program did, however, lead to a change in one monitored parameter used in PA: because of increased drilling in the Delaware Basin, the drilling rate parameter value used in the CRA-2009 PA has increased (see Appendix DATA-2009, Section DATA-2.0 for information on this parameter change).

In the CRA-2009 PA, the drilling rate has been changed to meet the requirements for 40 CFR § 194.33 (U.S. Environmental Protection Agency 1996). The drilling rate for boreholes is

discussed in Section 33 of this application. No changes to modeling assumptions are necessary to account for this parameter change.

MASS-2.3 Experimental Activities

The EPA requires the recertification documentation to include an update of "additional analyses and results of laboratory experiments conducted by the Department or its contractors as part of the WIPP program" (40 CFR § 194.15(a)(3); see also 40 CFR § 194.15, U.S. Environmental Protection Agency 1996). The following sections discuss analyses and experiments conducted to support compliance determinations. Only analyses with conclusions relevant to this recertification are discussed here.

MASS-2.3.1 Magnesium Oxide Investigations

The EPA has approved a U.S. Department of Energy (DOE) change request to reduce the magnesium oxide (MgO) excess factor from 1.67 to 1.2 times the quantity of MgO required to consume all of the carbon dioxide (CO_2) that would be produced if microbes consumed all the CPR materials in the emplaced waste at the WIPP (Reyes 2008 and Appendix MgO-2009, Section MgO-6.2.4.6). Since PA assumes there is always enough MgO to maintain a favorable chemical environment for actinide (An) solubilities, a reduction in the excess factor does not change the modeling assumptions used to represent MgO in PA.

Experiments have been performed to support the implementation of MgO as an engineered barrier. These experiments have characterized MgO and investigated the hydration and carbonization of MgO to confirm its ability to sequester CO_2, buffer brine pH, and subsequently help establish low An solubilities in the repository. These activities are described in detail in Appendix MgO-2009. The results of these MgO investigations have not impacted the modeling assumptions associated with MgO in PA (Appendix MgO-2009 and Appendix PA-2009, Section PA-2.1.4.4).

MASS-2.3.2 Actinide Investigations

The DOE has continued to investigate An speciation and solubilities since the certification of the WIPP. The current An experimental activities are described in Appendix SOTERM-2009, Section SOTERM-3.0. The CRA-2009 PA uses the same An assumptions as the CRA-2004 PABC.

MASS-2.4 Performance Assessment Models and Systems

Changes have been made to the systems used to perform PAs. The PA hardware, operating systems (OSs), and parameter database have been updated since the CRA-2004 and CRA-2004 PABC. These changes were necessary to replace obsolete hardware and OSs and to increase PA capabilities.

Sandia National Laboratories (SNL) maintains the computational platforms used to execute the WIPP PA modeling codes. A small number of modeling tasks that feed into compliance calculations are performed on desktop PC workstations running the Microsoft® Windows® XP

OS, as well as PC-based workstations and clusters running the Red Hat® Linux® OS. The WIPP PA parameter database is hosted on a PC-based server running Windows® 2000. However, the vast majority of the WIPP PA modeling codes used directly in compliance calculations are run on the WIPP PA Alpha Cluster composed of Hewlett Packard® (formerly Compaq®) AlphaServer™ systems. AlphaServers™ are built around the Alpha processor and run the OpenVMS™ OS.

The computer systems and OSs have been upgraded since the CRA-2004 because of increasing obsolescence of the OS and hardware. The current hardware and software versions used in the CRA-2009 PA calculations are shown in Table MASS-1 and Table MASS-2. Significant changes include those made to the WIPP PA Alpha cluster, where older AlphaServers™ were replaced with newer machines and the OS for all servers was upgraded. The WIPP PA Alpha cluster now consists of four ES47 AlphaServers™ and four ES45 AlphaServers™. The OS on these systems has been upgraded from OpenVMS™ 7.3-1 to OpenVMS™ 8.2. Regression testing of all codes used in compliance calculations has been performed to verify that the codes continue to perform correctly after the hardware and OS changes (Long 2006).

The PC-based Linux® clusters have also been upgraded since the CRA-2004, but the new configurations have not been used in compliance calculations included in the CRA-2009.

All changes to these systems are performed under the quality assurance (QA) program per the Carlsbad Field Office Quality Assurance Program Document, and include testing, validation, and verification to ensure that there is no impact on PA implementation. A synopsis of the changes and references to the QA documentation are found in Long (2006). It should be noted that the codes identified in Table 2-1 of Long (2006) are those that have changed since the CRA-2004 PABC. Some code outputs from previous certification PAs continue to be used in this CRA-2009 PA because these codes and their input parameters have not changed; therefore, the codes do not need to be rerun. These outputs are identified in Long (2008) and include the outputs of DRSPALL, MODFLOW, and SECOTP2D.

MASS-2.5 PABC

The EPA requested changes to the CRA-2004 PA during their review of the first recertification (Cotsworth 2005). These changes were incorporated in the CRA-2004 PABC and Leigh et al. (2005), and in the subsequent CRA-2009 PA. The changes were assessed by the EPA and approved as the certified WIPP baseline in their recertification decision (U.S. Environmental Protection Agency 2006). The CRA-2004 PABC changes are described in Table MASS-3.

MASS-2.5.1 Conceptual Model Changes

The CRA-2009 PA uses the same conceptual models used in the CRA-2004 PABC. No changes were made to the conceptual models used in the CRA-2004 PABC. For the CRA-2004 PABC, incorporation of the changes required by the EPA in Cotsworth (2005) led to several changes in the conceptual models used in the CRA-2004 PABC. Specifically, the requirement to assume that (1) microbial gas generation occurs for all vectors, and (2) the sequential consumption of CPR via the nitrate-to-sulfate-to-methanogenesis reaction sequence is constrained to limit the

Table MASS-1. CRA-2009 PA Codes

Code	Version	Build Date
ALGEBRACDB	2.35	31-JAN-1996
BRAGFLO	6.0	12-FEB-2007
CCDFGF	5.02	13-DEC-2004
CUTTINGS_S	6.02	9-JUN-2005
DRSPALL	1.10	14-JAN-2004
EPAUNI	1.15A	3-JUL-2003
GENMESH	6.08	31-JAN-1996
GROPECDB	2.12	27-JUN-1996
ICSET	2.22	1-FEB-1996
LHS	2.42	18-JAN-2005
MATSET	9.10	29-NOV-2001
MODFLOW-2000	1.6	20-SEP-2002
NUTS	2.05C	24-MAY-2006
PANEL	4.03	25-APR-2005
POSTBRAG	4.00A	28-MAR-2007
POSTSECOTP2D	1.04	5-JUN-1997
POSTLHS	4.07A	25-APR-2005
PREBRAG	8.0	8-MAR-2007
PRECCDFGF	1.01	7-JUL-2005
PRELHS	2.30	27-NOV-2001
PRESECOTP2D	1.22	12-JUN-1997
RELATE	1.43	6-MAR-1996
SECOTP2D	1.41A	9-JUL-2003
STEPWISE	2.21	2-DEC-1996
SUMMARIZE	3.01	21-DEC-2005

Table MASS-2. CRA-2009 PA Hardware

Node	Hardware Type	CPU
CCR	HP AlphaServer™ ES45	Alpha EV68
TDN	HP AlphaServer™ ES45	Alpha EV68
BTO	HP AlphaServer™ ES45	Alpha EV68
CSN	HP AlphaServer™ ES45	Alpha EV68
GNR	HP AlphaServer™ ES47	Alpha EV7
MC5	HP AlphaServer™ ES47	Alpha EV7
TRS	HP AlphaServer™ ES47	Alpha EV7
TBB	HP AlphaServer™ ES47	Alpha EV7

consumption reaction to only nitrate and sulfate reduction, changed the chemical conditions and gas generation conceptual models for the CRA-2004 PABC. These changes are also incorporated in the CRA-2009 PA and are discussed further in the CRA-2004 PABC summary report sections listed in Table MASS-3.

Table MASS-3. Changes Incorporated in the CRA-2004 PABC

Changes Included in the Performance Assessment Baseline Calculation		
EPA-Mandated Change	**Description of Change**	**Reference**
Solubility Parameters	Organic ligand concentrations recalculated, brine composition changes, U(VI) solubility changes, and change to account for no nonmicrobial vectors	PABC Summary (Leigh et al. 2005, Section 2.5) PANEL Analysis Package (Garner and Leigh 2005)
Solubility Uncertainty Ranges	Updated uncertainty ranges used	PABC Summary (Leigh et al. 2005, Section 2.6)
Probability of Microbial Activity	Microbial activity in all vectors versus 50% previously	PABC Summary (Leigh et al. 2005, Section 2.2)
CPR Degradation	Parameters for humid and inundated rate-changed Removal of methanogenesis	PABC Summary (Leigh et al. 2005, Section 2.3) PABC Summary (Leigh et al. 2005, Section 2.4)
Inventory	Inclusion of waste emplacement CPR Correct inventory errors	PABC Summary (Leigh et al. 2005, Section 2.1) PABC Inventory Report (Leigh, Trone, and Fox 2005)
Error Corrections	Additional DRSPALL vectors sampled; LHS, CCDFGF, CUTTING_S, SUMMARIZE and PRECCDFGF code corrections	PABC Summary (Leigh et al. 2005, Section 2.8) PABC Summary (Leigh et al. 2005, Section 2.9)
Culebra T Fields	Mining modifications incorporated in new flow fields	PABC Summary (Leigh et al. 2005, Section 2.7) The CRA-2004, Appendix PA, Attachment TFIELD

MASS-2.5.2 Recalculation of Culebra T Fields

The CRA-2009 PA uses the CRA-2004 PABC T fields. No changes were made to the T field modeling assumptions for the CRA-2009 PA. Water level rises in the Culebra Dolomite Member of the Rustler Formation (hereafter referred to as Culebra) have continued over recent years, and the observed heads have exceeded the ranges of uncertainty established for the steady-state heads in many of the WIPP observation wells used in the calibration of the T fields described in the CCA (Sandia National Laboratories 2002). The DOE recalculated T fields for the CRA-2004 using new Culebra data and geologic information (see Appendix TFIELD-2009). Additionally, the treatment of potential potash mining was recalculated during the CRA-2004 PABC. The areas affected by mining were modified, and new flow fields were generated in response to the EPA's request for a PABC (Cotsworth 2005). (See also Leigh et al 2005, Section

2.7, and the CRA-2004, Appendix PA, Attachment TFIELD.) The DOE is continuing its field observation program to investigate other potential causes for the water-level rises (Sandia National Laboratories 2003). This program is discussed in Appendix HYDRO-2009.

MASS-2.5.3 Waste Inventory Update

The waste inventory used in the CCA was based on information contained in the Transuranic Waste Baseline Inventory Database (see the CCA, Appendix BIR). No waste had been emplaced in the repository at that time. Since 1996, waste has been emplaced in the repository and better estimates have been made of the existing and projected waste streams at the generator sites. Waste information in the CRA-2004 PA was updated to include the emplaced, currently stored, and projected waste streams. This information was collected in the Transuranic Waste Baseline Inventory Database, Rev 2.1, with the WIPP-specific information detailed in the CRA-2004, Appendix DATA, Attachment F.

During the CRA-2004 PABC, the inventory information used in PA was again updated. Leigh, Trone, and Fox (2005) summarizes these changes to the inventory. Changes include a correction to the waste volumes reported by the Hanford Office of Richland Operations, the inclusion of pre-1970 waste at Idaho National Laboratory (INL) as possible WIPP waste and a correction to the volume and concentration of waste from Los Alamos National Laboratory.

The waste information used in the CRA-2009 PA is the same as in the CRA-2004 PABC calculations, with the addition of cellulosic and plastic materials used for waste emplacement to the inventory. Waste information in the CRA-2009 PA is discussed further in Leigh, Trone, and Fox (2005).

MASS-2.6 CRA-2009 Changes

The CRA-2009 PA was updated based on new information since the CRA-2004 PABC. Information on the implementation of these changes is contained in Clayton (2008, Section 2.1) and is summarized in Table MASS-4.

MASS-2.7 Operational Considerations

No operational changes that would impact modeling assumptions have been made at the WIPP since the 2006 recertification decision. As a result, no changes were made to modeling assumptions for the CRA-2009 PA.

Shortly after submission of the CRA-2004 to the EPA, the DOE began using a new MgO supplier, Martin Marrietta Magnesia Specialties, for the engineered barrier because the existing vendor, Premier Chemicals, was no longer able to meet the stipulated MgO specifications. The MgO specification did not change, and no associated change was made to modeling assumptions as a result of the new vendor. Additional discussion of this operational change is found in Appendix MgO-2009, Section MgO-2.2.

Table MASS-4. Changes Incorporated in the CRA-2009

WIPP Project Change	Summary of Change and Cross-Reference
DBR Parameters	The maximum DBR duration was decreased from 11 days to 4.5 days (Kirkes 2007).
CPR Degradation Rates	A conditional relationship was introduced between the inundated and humid gas generation rate to ensure that the inundated rate is the maximum rate (Kirchner 2008).
BRAGFLO Chemistry Capillary Pressure and Relative Permeability Model	New capillary pressure and relative permeability model for open cavities was added. Cut-off saturation is used, below which no chemical reactions occur (H_2O-required reactions) (Nemer and Clayton 2008).
Drilling Rate	Rate changed from 52.5 to 58.5 boreholes per square kilometer (km^2) over 10,000 years (Clayton 2008).
Parameter Error Corrections	Emplaced CPR Error Correction Halite/DRZ Porosity Error Correction Fraction of Repository Occupied by Waste Correction NUTS and DBR Calculation Input Files (Nemer 2007, Dunagan 2007, Ismail 2007a, Ismail 2007b, Clayton 2007).

MASS-3.0 General Assumptions in PA Models

A number of assumptions are applied generally to the disposal system through the conceptual and mathematical models implemented in the CRA-2009 PA.

Table MASS-5, which lists modeling assumptions used in the PA, is a guide to general modeling assumptions and provides guidance for integrating the assumptions with (1) the CRA-2004 chapters or CRA-2009 appendices in which they are discussed, and (2) the code(s) that implement these assumptions.

The FEPs discussed in Appendix SCR-2009 that are relevant to these assumptions are also indicated. The final column in the table indicates whether the DOE considers each assumption to be reasonable or conservative. As discussed in the CRA-2004, Chapter 6.0, Section 6.5, the DOE has not attempted to bias the overall results of PA toward a conservative outcome. However, where data or models are impractical to obtain, or where effects on performance are not expected to be significant enough to justify development of a more complicated model, the DOE has chosen to use conservative assumptions. In all other cases, best unbiased conceptual models and parameter values have been selected. The designator R (reasonable) in the final column indicates that the DOE considers the assumption to be reasonable based on WIPP-specific data or information, data or information considered analogous to the WIPP disposal system, expert judgment, or other reasoning. The designator C (conservative) indicates the DOE considers the assumption may overestimate a process or effect that may contribute to releases to the accessible environment. The regulatory designator (Reg) indicates that the assumption is based on regulations in 40 CFR Part 191, criteria in 40 CFR Part 194, or other regulatory guidance.

MASS-3.1 Darcy's Law Applied to Fluid Flow Calculated by BRAGFLO, MODFLOW-2000, and DRSPALL

A mathematical relationship expressing fluid flux as a function of hydraulic head gradients in a porous medium, commonly known as Darcy's Law, is applied to geologic media for all fluid-flow calculations. For details about the specific formulation of Darcy's Law used in these calculations, refer to Appendix PA-2009, Section PA-4.2 for the disposal system and Section PA-4.8 for the Culebra. Darcy's Law is not applied for flow up a borehole being drilled (see Section MASS-16.2; the CRA-2004, Chapter 6.0, Section 6.4.7.1.1; and Appendix PA-2009, Section PA-4.6 for more discussion of this topic).

Darcy's Law generally applies for flow models if certain conditions are satisfied: (1) the flow occurs in a porous medium with interconnected porosity, (2) flow velocities are low enough that viscous forces dominate inertial forces, and (3) a threshold hydraulic gradient is exceeded. In the CCA, Appendix MASS, these conditions were shown to be valid for the WIPP PA.

Darcy's Law assumes laminar flow; that is, there is no motion of the fluid at the fluid/solid interface and velocity increases with distance from the fluid/solid interface. For liquids, it is reasonable to assume laminar flow under most conditions, including those found in and surrounding the WIPP repository. For gases at low pressure, however, gas molecules near the solid interface may not have intimate contact with the solid and may have finite velocity, not

Table MASS-5. General Modeling Assumptions

Chapter or Section	Assumption Number	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
MASS-3.0 Some General Assumptions in PA Models MASS-3.1 Darcy's Law Applied for Fluid Flow calculated by BRAGFLO, MODFLOW-2000, and SECOTP2D	1	BRAGFLO MODFLOW-2000	Flow is governed by mass conservation and Darcy's Law in porous media. Flow is laminar and fluids are Newtonian.	Saturated Groundwater Flow (N23) Unsaturated Groundwater Flow (N24) Brine Inflow (W40)	R
	2	BRAGFLO	Two-phase flow in the porous media is by simultaneous immiscible displacement.	Fluid Flow Due to Gas Production (W42)	R
	3	BRAGFLO	The Brooks-Corey or Van Genuchten/Parker equations represent interactions between brine and gas.	Fluid Flow Due to Gas Production (W42)	R
	4	BRAGFLO	The Klinkenberg effect is included for flow of gases at low pressures.	Fluid Flow Due to Gas Production (W42)	R
	5	BRAGFLO	Threshold displacement pressure for flow of gas into brine is constant.	Fluid Flow Due to Gas Production (W42)	R
	6	BRAGFLO MODFLOW-2000 SECOTP2D	Fluid composition and compressibility are constant.	Saturated Groundwater Flow (N23) Fluid Flow Due to Gas Production (W42)	R
MASS-3.2 Hydrogen Gas as Surrogate for Waste-Generated Gas Physical Properties in BRAGFLO	7	BRAGFLO DRSPALL	The gas phase is assigned the density and viscosity properties of hydrogen.	Fluid Flow Due to Gas Production (W42)	R
MASS-3.3 Salado Brine as Surrogate for Liquid Phase Physical Properties in BRAGFLO	8	BRAGFLO	All liquid physical properties are assigned the properties of Salado brine.	Saturated Groundwater Flow (N23)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance

See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.2 Model Geometries MASS-4.0 Model Geometries CRA-2004, Chapter 6.0, Section 6.4.2.1 Disposal System Geometry MASS-4.1 Disposal System Geometry as Modeled in BRAGFLO	BRAGFLO	The disposal system is represented by a two-dimensional, north-south, vertical cross section.	Stratigraphy (N1) Physiography (N39)	R
	BRAGFLO	Flow in the disposal system is radially convergent or divergent centered on the repository, shaft, and borehole for disturbed performance.	Saturated Groundwater Flow (N23) Unsaturated Groundwater Flow (N24)	R
	BRAGFLO	Variable dip in the Salado is approximated by a 1 degree dip to the south.	Stratigraphy (N1)	R
	BRAGFLO	Stratigraphic layers are parallel.	Stratigraphy (N1)	R
	BRAGFLO	The stratigraphy consists of units above the Dewey Lake, the Forty-niner, the Magenta, the Tamarisk, the Culebra, the Los Medaños, and the Salado Formations (comprising impure halite, MB 138, anhydrites A and B [lumped together], and MB 139). The dimensions of these units are constant. A Castile brine reservoir is included in the BRAGFLO grid in all scenarios.	Stratigraphy (N1)	R
CRA-2004, Chapter 6.0, Section 6.4.2.2 Culebra Geometry MASS-4.3 Historical Context of Culebra Geometries as Modeled in MODFLOW-2000 and SECOTP2D	MODFLOW-2000 SECOTP2D	The Culebra is represented by a two-dimensional, horizontal geometry for groundwater flow and radionuclide transport simulation.	Stratigraphy (N1)	R
	MODFLOW 2000 PEST	Transmissivity varies spatially. There is no vertical flow to or from the Culebra.	Groundwater Recharge (N54) Groundwater Discharge (N53)	R
	SECOTP2D	The regional flow field provides boundary conditions for local transport calculations (see CRA-2004, Chapter 6.0, Section 6.4.10.2).	Advection (W90)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

1

Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.3 The Repository MASS-5.0 BRAGFLO Geometry of the Repository	BRAGFLO	The repository comprises five regions separated by panel closures: the waste panel, a north Rest of Repository (RoR), a south RoR and the access drifts (separated by panel closures), the operations region, and the experimental region. A single shaft region is also modeled, and a borehole region is included for a borehole that intersects the separate waste panel. The dimensions of these regions are constant (see the CRA-2004, Appendix MASS, Figure MASS-4).	Disposal Geometry (W1)	R-C
	BRAGFLO	Long-term flow up plugged and abandoned boreholes modeled as if all intrusions occur into a downdip (southern) panel.	Disposal Geometry (W1)	C
	BRAGFLO	For each repository region, the model geometry preserves design volume.	Disposal Geometry (W1)	R
	BRAGFLO	Pillars, individual drifts, and rooms are not modeled for long-term performance, and containers provide no barrier to fluid flow.	Disposal Geometry (W1)	C
	BRAGFLO	Long-term flow is radial to and from the borehole that intersects the waste disposal panel during disturbed performance.	Waste-Induced Borehole Flow (H32)	R
	BRAGFLO	DRZ provides a pathway to MBs.	—	R
	BRAGFLO	Grid and material properties are consistent with the Option D panel closure design.	—	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.3.1 Creep Closure MASS-6.0 Creep Closure Appendix PORSURF	SANTOS	Creep closure is modeled using a two-dimensional model of a single room. Room interactions are insignificant.	Salt Creep (W20) Changes in the Stress Field (W21) Excavation-Induced Changes in Stress (W19)	R
	SANTOS	The amount of creep closure is a function of time, gas pressure, and waste-matrix strength.	Salt Creep (W20) Changes in the Stress Field (W21) Consolidation of Waste (W32) Pressurization (W26)	R
	BRAGFLO	Porosity of operations and experimental areas is fixed at a value representative of consolidated material.	Salt Creep (W20)	R
CRA-2004, Chapter 6.0, Section 6.4.3.2 Repository Fluid Flow MASS-7.0 Repository Fluid Flow	BRAGFLO	General assumptions 1 to 8.	—	See above
	BRAGFLO	The waste disposal region is assigned a constant permeability representative of average consolidated waste without backfill.	Saturated Groundwater Flow (N23) Unsaturated Groundwater Flow (N24)	R
MASS-7.1 Flow Interactions with the Creep Closure Model	BRAGFLO	The experimental and operations regions are assigned a constant permeability representative of unconsolidated material and a constant porosity representative of consolidated material.	Saturated Groundwater Flow (N23) Unsaturated Groundwater Flow (N24) Salt Creep (N20)	C
MASS-7.2 Flow Interactions with the Gas Generation Model	BRAGFLO	For gas generation calculations, the effects of wicking are accounted for by assuming that brine in the repository contacts waste to an extent greater than that calculated by the Darcy Flow model used.	Wicking (W41)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.3.3 Gas Generation MASS-8.0 Gas Generation CRA-2004 Appendix TRU WASTE	BRAGFLO	Gas generation occurs by anoxic corrosion of steel containers and Fe and Fe-base alloys in the waste, giving H_2, and by microbial consumption of cellulosics and, possibly, plastics and rubbers, giving mainly CO_2 and H_2S. Radiolysis, oxic reactions, and other gas generation mechanisms are insignificant. Gas generation is calculated using the average-stoichiometry model, and is dependent on brine availability.	Container Material Inventory (W5) Waste Inventory (W2) Degradation of Organic Material (W44) Gases from Metal Corrosion (W49)	R
	BRAGFLO	The anoxic corrosion rate is dependent on liquid saturation. Anoxic corrosion of steel continues until all the steel is consumed. Steel corrosion will not be passivated by microbially generated gases (CO_2 or H_2S). The water in brine is consumed by the corrosion reaction.	Brine Inflow (W40) Gases from Metal Corrosion (W49) Degradation of Organic Material (W44)	R
	BRAGFLO	Laboratory-scale experimental measurements of gas generation rates at expected room temperatures are used to account for the effects of biofilms and chemical reactions.	Effects of Biofilms on Microbial Gas Generation (W48) Effects of Temperature on Microbial Gas Generation (W45) Chemical Effects of Corrosion (W51)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	BRAGFLO	The rate of microbial gas production is dependent on the amount of liquid present. It is assumed that microbial activity neither produces nor consumes water. Significant microbial activity occurs in all the simulations. In 75% of the simulations, microbes may consume all of the cellulosics but none of the plastics and rubbers. In the remaining 25% of the simulations, microbes may consume all of the cellulosics and all of the plastics and rubbers. Microbial production will continue until all biodegradable CPR materials are consumed if brine is present. The MgO backfill will react with all of the CO_2 and remove it from the gaseous phase.	Brine Inflow (W40) Degradation of Organic Material (W44) Waste Inventory (W2)	R
	BRAGFLO	Gas dissolution in brine is of negligible consequence.	Fluid Flow Due to Gas Production (W42)	R
	BRAGFLO	The gaseous phase is assigned the properties of hydrogen (General Assumption 7).	Fluid Flow Due to Gas Production (W42)	See above
CRA-2004, Chapter 6.0, Section 6.4.3.4 Chemical Conditions in the Repository SOTERM-2.0 Conceptual Framework of Chemical Conditions	NUTS PANEL	Chemical conditions in the repository will be constant. Chemical equilibrium is assumed for all reactions that occur between brine in the repository, waste, and abundant minerals, with the exceptions of gas generation and redox reactions.	Speciation (W56) Reduction-Oxidation Kinetics (W66)	R
	NUTS PANEL	Brine and waste in the repository will contain a uniform mixture of dissolved and colloidal species. All actinides have instant access to all repository brine.	Heterogeneity of Waste Forms (W3) Speciation (W56)	C

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	NUTS PANEL	No microenvironments that influence the overall chemical environment will persist.	Speciation (W56)	R
	NUTS PANEL	For the undisturbed performance and E2 scenarios, brine in the waste panels has the composition of Salado brine. For E1 and E1E2 (Appendix PA-2009, Section PA-2.3.2.2) scenarios, all brine in the waste panel intersected by the borehole has the composition of Castile brine.	Speciation (W56)	R
	NUTS PANEL	Chemical conditions in the waste panels will be reducing. However, a condition of redox disequilibrium will exist between the possible oxidation states of the An elements.	Reduction-Oxidation Kinetics (W66) Speciation (W56) Effects of Metal Corrosion (W64)	R
	NUTS PANEL	The pH and CO_2 fugacity in the waste panels will be controlled by the equilibrium between $Mg(OH)_2$ and $Mg_5(CO_3)_4(OH)_2{\cdot}4H_2O$. (A result of this assumption is low CO_2 fugacity and mildly basic conditions.)	Speciation (W56) Backfill Chemical Composition (W10)	R
CRA-2004, Chapter 6.0, Section 6.4.3.5 Dissolved Actinide Source Term SOTERM-3.3 The Fracture Matrix Transport Computer Code	NUTS PANEL	Radionuclide dissolution to solubility limits is instantaneous.	Dissolution of Waste (W58)	C
	NUTS PANEL	Of the 29 isotopes considered as inputs, 6 actinides (Th, U, Np, Pu, Am, and Cm) are used in PANEL for calculations of radionuclide transport of brine (up a borehole). Four actinides (Th, U, Pu, and Am) are explicitly considered in NUTS for calculations of radionuclide transport in brine (porous materials) (Leigh and Trone 2005a). Choice of radionuclides is discussed in Leigh and Trone (2005b), Leigh, Trone, and Fox (2005), and Leigh et al. (2005).	Waste Inventory (W2)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	NUTS PANEL	The reducing conditions in the repository will eliminate significant concentrations of Np(VI), Pu(V), Pu(VI), and Am(V) species. Am and Cm will exist predominantly in the III oxidation state; while Th will exist in the IV oxidation state. It is assumed that the solubilities and K_ds of U, Np, and Pu will be dominated by one of the remaining oxidation states: U(IV) or U(VI), Np(IV) or Np(V), and Pu(III) or Pu(IV) (See Appendix SOTERM-2009, Table SOTERM-15).	Speciation (W56) Reduction-Oxidation Kinetics (W66)	R
	NUTS PANEL	For a given oxidation state, the different actinides have similar solubilities.	Speciation (W56)	R
	NUTS PANEL	For undisturbed performance and for all aspects of disturbed performance, except for cuttings and cavings releases, radionuclides in the waste are distributed evenly throughout the disposal panel.	Waste Inventory (W2) Heterogeneity of Waste Forms (W3)	R
	NUTS PANEL	Mobilization of actinides in the gas phase is negligible.	Dissolution of Waste (W58)	R
	NUTS PANEL	An concentrations in the repository will be inventory limited when the mass of an An becomes depleted such that the predicted concentrations cannot be achieved.	Dissolution of Waste (W58)	R
CRA-2004, Chapter 6.0, Section 6.4.3.6 Source Term for Colloidal Actinides	NUTS PANEL	Four types of colloids constitute the source term for colloidal actinides: microbes, humic substances, intrinsic colloids, and mineral fragments.	Colloid Formation and Stability (W79) Humic and Fulvic Acids (W70)	R
	NUTS PANEL	The only intrinsic colloids that will form are those of Pu.	Colloid Formation and Stability (W79)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	NUTS PANEL	Concentrations of intrinsic colloids and mineral-fragment colloids are modeled as constants based on experimental observations. Humic and microbial colloidal An concentrations are modeled as proportional to dissolved An concentrations.	Colloid Formation and Stability (W79)	R
	NUTS PANEL	The maximum concentration of each An associated with each colloid type is constant.	Actinide Sorption (W61)	R
CRA-2004, Chapter 6.0, Section 6.4.4 Shafts and Shaft Seals MASS-12.0 Shafts and Shaft Seals	BRAGFLO	General Assumptions 1 to 8.	—	See above
	BRAGFLO	The four shafts connecting the repository to the surface are represented by a single shaft with a cross-section and volume equal to the total volume of the four real shafts and separated from the waste by less than the distance of the nearest real shaft.	Disposal Geometry (W1)	R
	BRAGFLO	The shaft seal system is represented by an upper and lower shaft region representing a composite of the actual materials in those regions.	Shaft Seal Geometry (W6) Shaft Seal Physical Properties (W7)	R
	BRAGFLO	The shaft is surrounded by a DRZ which heals with time. The DRZ is represented through the composite permeabilities of the shaft system itself, rather than as a discrete zone. The effective permeability of shaft materials are adjusted at 200 years after closure to reflect consolidation and possible degradation. Permeabilities are constant for the shaft seal materials through the Rustler formation.	Salt Creep (W20) Consolidation of Shaft Seals (W36) DRZ (W18) Microbial Growth on Concrete (W76) Chemical Degradation of Shaft Seals (W74) Mechanical Degradation of Shaft Seals (W37)	R
	BRAGFLO	Concrete shaft components of the lower shaft are modeled as if they degrade after emplacement.	Mechanical Degradation of Shaft Seals (W37)	C

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
1 See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	NUTS	Radionuclides are not retarded by the seals.	Actinide Sorption (W61) Speciation (W56)	C
CRA-2004, Chapter 6.0, Section 6.4.5 The Salado MASS-13.0 Salado	BRAGFLO	General Assumptions 1 to 8.	—	See above
CRA-2004, Chapter 6.0, Section 6.4.5.1 Impure Halite MASS-13.1 High Threshold Pressure for Halite-Rich Salado Rock Units	BRAGFLO	Intact rock and hydrologic properties are constant.	Stratigraphy (N1)	R
CRA-2004, Chapter 6.0, Section 6.4.5.2 Salado Interbeds MASS-13.3 The Fracture Model	BRAGFLO	Interbeds have a fracture-initiation pressure above which local fracturing and changes in porosity and permeability occur in response to changes in pore pressure. A power function relates the permeability increase to the porosity increase. A pressure is specified above which porosity and permeability do not change.	Disruption Due to Gas Effects (W25)	R
	BRAGFLO	Interbeds have identical physical properties; they differ only in position, thickness, and some fracture parameters.	Saturated Groundwater Flow (N23)	R
CRA-2004, Chapter 6.0, Section 6.4.5.3 Disturbed Rock Zone MASS-13.4 Flow in the Disturbed Rock Zone	BRAGFLO	The permeability of the DRZ is sampled with the low value similar to intact halite and the high value representing a fractured material. The DRZ porosity is equal to the porosity of Salado halite to plus 0.29%.	Disturbed Rock Zone (DRZ) (W18) Roof Falls (W22) Gas Explosions (W27) Seismic Activity (N12) Underground Boreholes (W39)	C-R
CRA-2004, Chapter 6.0, Section 6.4.5.4 Actinide Transport in the Salado MASS-13.5 Actinide Transport in the Salado	NUTS	Dissolved actinides and colloidal actinides are transported by advection in the Salado. Diffusion and dispersion are assumed negligible.	Advection (W90) Diffusion (W91) Matrix Diffusion (W92)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	NUTS	Sorption of actinides in the anhydrite interbeds, colloid retardation, colloid transport at higher than average velocities, coprecipitation of minerals containing actinides, channeled flow, and viscous fingering are not modeled.	Actinide Sorption (W61) Colloid Transport (W78) Colloid Filtration (W80) Colloid Sorption (W81) Fluid Flow Due to Gas Production (W42) Fracture Flow (N25)	R
	NUTS	Radionuclides having similar decay and transport properties have been grouped together for transport calculations as discussed in Leigh and Trone (2005a). See also assumptions for dissolved actinide source term.	Radionuclide Decay and Ingrowth (W12)	R
	NUTS	Sorption of actinides in the borehole is not modeled.	Actinide Sorption (W61)	C
CRA-2004, Chapter 6.0, Section 6.4.6 Units Above the Salado MASS-14.0 Geologic Units above the Salado	SECOTP2D	Above the Salado, lateral An transport to the accessible environment can occur only through the Culebra.	Saturated Groundwater Flow (N23) Unsaturated Groundwater Flow (N24) Solute Transport (W77)	R
CRA-2004, Chapter 6.0, Section 6.4.6.1 Los Medaños	MODFLOW-2000 BRAGFLO	The Los Medaños member of the Rustler Formation, Tamarisk, and Forty-niner are assumed to be impermeable.	Saturated Groundwater Flow (N23)	C
CRA-2004, Chapter 6.0, Section 6.4.6.2 The Culebra MASS-15.0 Culebra Appendix TFIELD	MODFLOW-2000 SECOTP2D	General Assumptions 1, 6, and 8.	—	See above
	MODFLOW-2000	For fluid flow, the Culebra is modeled as a uniform (single-porosity) porous medium.	Saturated Groundwater flow (N23)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	MODFLOW-2000	The Culebra flow field is determined from the observed hydraulic conditions and estimates of the effects of climate change and potash mining outside the controlled area, and does not change with time unless mining is predicted to occur in the disposal system in the future.	Saturated Groundwater Flow (N23) Climate Change (N61) Precipitation (e.g.,, Rainfall) (N59) Temperature (N60) Changes in Groundwater Flow Due to Mining (H37)	R
	BRAGFLO	The Culebra is assigned a single permeability to calculate brine flow into the unit from an intrusion borehole.	Natural Borehole Fluid Flow (H31) Waste-Induced Borehole Flow (H32)	R
	MODFLOW-2000	Gas flow in the Culebra is not modeled. Gas from the repository does not affect fluid flow in the Culebra.	Saturated Groundwater Flow (N23) Fluid Flow Due to Gas Production (W42)	R
	BRAGFLO MODFLOW-2000 SECOTP2D	Different thicknesses of the Culebra are assumed for BRAGFLO, MODFLOW-2000, and SECOTP2D calculations, although the Ts are consistent.	Effects of Preferential Pathways (N27)	R
	PEST	Uncertainty in the spatial variability of the Culebra transmissivity is accounted for by statistically generating 100 T fields for PA.	Saturated Groundwater Flow (N23) Fracture Flow (N25) Shallow Dissolution (N16)	R
	MODFLOW-2000 BRAGFLO	Potentiometric heads are set on the edges of the regional grid to represent flow in a portion of a much larger hydrologic system.	Groundwater Recharge (N54) Groundwater Discharge (N53) Changes in Groundwater Recharge and Discharge (N56) Infiltration (N55)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.6.2.1 Transport of Dissolved Actinides in the Culebra MASS-15.2 Dissolved Actinide Transport and Retardation in the Culebra	SECOTP2D	Dissolved actinides are transported by advection in high-permeability features and by diffusion in low-permeability features.	Solute Transport (W77) Advection (W90) Diffusion (W91) Matrix Diffusion (W92)	R
	SECOTP2D	Sorption occurs on dolomite in the matrix. Sorption on clays present in the Culebra is not modeled.	Actinide Sorption (W61) Changes in Sorptive Surfaces (W63)	C
	SECOTP2D	Sorption is represented using a linear isotherm model.	Actinide Sorption (W61) Kinetics of Sorption (W62)	R
	SECOTP2D	The possible effects on sorption of the injection of brines from the Castile and Salado into the Culebra are accounted for in the distribution of An K_ds.	Actinide Sorption (W61) Groundwater Geochemistry (N33) Changes in Groundwater Eh (N36) Changes in Groundwater pH (N37) Natural Borehole Fluid Flow (H31)	R
	SECOTP2D	Hydraulically significant fractures are assumed to be present everywhere in the Culebra.	Advection (W90)	C
CRA-2004, Chapter 6.0, Section 6.4.6.2.2 Transport of Colloidal Actinides in the Culebra MASS-15.3 Colloidal Actinide Transport and Retardation in the Culebra	SECOTP2D	An humic colloids are chemically retarded identically to dissolved actinides and are treated as dissolved actinides.	Advection (W90) Diffusion (W91) Colloid Transport (W78) Microbial Transport (W87)	R
	SECOTP2D	The concentration of intrinsic colloids is sufficiently low to justify elimination from PA transport calculations in the Culebra.	—	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	SECOTP2D	Microbial colloids and mineral fragments are too large to undergo matrix diffusion. Filtration of these colloids, which is modeled using an exponential decay approach, occurs in high-permeability features. Attenuation is so effective that associated actinides are assumed to be retained within the disposal system and are not transported in SECOTP2D.	Microbial Transport (W87) Colloid Sorption (W81)	R
CRA-2004, Chapter 6.0, Section 6.4.6.2.3 Subsidence Due to Potash Mining MASS-15.4 Subsidence Caused by Potash Mining in the Culebra	MODFLOW-2000	The effect of potash mining is to increase the hydraulic conductivity in the Culebra by a factor between 1 and 1,000.	Conventional Underground Potash Mining (H13) Changes in Groundwater Flow Due to Mining (H37)	Reg.
CRA-2004, Chapter 6.0, Section 6.4.6.3 The Tamarisk	MODFLOW-2000 BRAGFLO	The Tamarisk is assumed to be impermeable.	Saturated Groundwater Flow (N23)	R
CRA-2004, Chapter 6.0, Section 6.4.6.4 The Magenta	BRAGFLO	General Assumptions 1 to 8.	—	See above
	BRAGFLO	The Magenta permeability is set to the lowest value measured near the center of the WIPP site. This increases the flow into the Culebra.	Saturated Groundwater Flow (N23)	R
	NUTS	No radionuclides entering the Magenta will reach the accessible environment. However, the volumes of brine and actinides entering and stored in the Magenta are modeled.	Solute Transport (W77)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.6.5 The Forty-niner	BRAGFLO	The Forty-niner is assumed to be impermeable.	Saturated Groundwater Flow (N23)	R
CRA-2004, Chapter 6.0, Section 6.4.6.6 Dewey Lake	BRAGFLO	General Assumptions 1 to 8.	—	See above
	NUTS	The sorptive capacity of the Dewey Lake is sufficiently large to prevent any release over 10,000 years.	Saturated Groundwater Flow (N23) Actinide Sorption (W61)	R
CRA-2004, Chapter 6.0, Section 6.4.6.7 Supra-Dewey Lake Units	BRAGFLO	General Assumptions 1 to 8.	—	See above
	BRAGFLO	The units above the Dewey Lake are a single hydrostratigraphic unit.	Stratigraphy (N1)	R
	BRAGFLO	The units are thin and predominantly unsaturated.	Unsaturated Groundwater Flow (N24) Saturated Groundwater Flow (N23)	R
CRA-2004, Chapter 6.0, Section 6.4.7 The Intrusion Borehole MASS-16.0 Intrusion Borehole CRA-2004 Section 6.4.7.1 Releases during Drilling	CUTTINGS_S BRAGFLO DRSPALL	Any actinides that enter the borehole during drilling are assumed to reach the surface.	—	C
MASS-16.1 Cuttings, Cavings, and Spall Releases during Drilling	BRAGFLO PANEL CUTTINGS_S DRSPALL	Future drilling practices will be the same as they are at present.	Oil and Gas Exploration (H1) Potash Exploration (H2) Oil and Gas Exploitation (H4) Other Resources (H8) Enhanced Oil and Gas Recovery (H9)	Reg.
	CUTTINGS_S DRSPALL	Releases of particulate waste material are modeled (cuttings, cavings, and spallings). Releases are corrected for radioactive decay until the time of intrusion.	Drilling Fluid Flow (H21) Suspension of Particles (W82) Cuttings (W84) Cavings (W85) Spallings (W86)	R
	CUTTINGS_S	Degraded waste properties are based on marine clays and surrogate materials.	Cavings (W85)	C

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
1 See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	DRSPALL	A hemispherical geometry with one-dimensional spherical symmetry defines the flow field and cavity in the waste.	Spallings (W86)	C
	DRSPALL	Tensile strength, based on completely degraded waste surrogates, is felt to represent extreme, low-end tensile strengths because it does not account for several strengthening mechanisms.	Spallings (W86)	C
	DRSPALL	Shape factor is 0.1, corresponding to particles that are easier to fluidize and entrain in the flow.	Spallings (W86)	C
CRA-2004, Chapter 6.0, Section 6.4.7.1.1 Direct Brine Release During Drilling MASS-16.2 Direct Brine Releases during Drilling	BRAGFLO PANEL	Brine containing actinides may flow to the surface during drilling. DBR will have negligible effect on the long-term pressure and saturation in the waste panel.	Blowouts (H23)	R
	BRAGFLO	A two-dimensional grid (one degree dip) on the scale of the waste disposal region is used for DBR calculations.	Blowouts (H23)	R
	BRAGFLO CCDFGF	Calculation of DBR from several different locations provides reference results for the variation in release associated with location.	Blowouts (H23)	R
CRA-2004, Chapter 6.0, Section 6.4.7.2 Long-Term Releases Following Drilling MASS-16.3 Long-Term Properties of the Abandoned Intrusion Borehole	BRAGFLO CCDFGF	Plugging and abandonment of future boreholes are assumed to be consistent with practices in the Delaware Basin.	Natural Borehole Fluid Flow (H31) Waste-Induced Borehole Flow (H32)	Reg.
CRA-2004, Chapter 6.0, Section 6.4.7.2.1 Continuous Concrete Plug through the Salado and Castile	BRAGFLO CCDFGF	A continuous concrete plug is assumed to exist throughout the Salado and Castile. Long-term releases through a continuous plug are analogous to releases through a sealed shaft.	Natural Borehole Fluid Flow (H31) Waste-Induced Borehole Flow (H32)	Reg.-R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.7.2.2 The Two-Plug Configuration	BRAGFLO	A lower plug is located between the Castile brine reservoir and underlying formations. A second plug is located immediately above the Salado. The brine reservoir and waste panel are in direct communication though an open cased hole.	Natural Borehole Fluid Flow (H31) Waste-Induced Borehole Flow (H32)	Reg.-R
	BRAGFLO	The casing and upper concrete plug are assumed to fail after 200 years, and the borehole is assumed to be filled with silty-sand-like material. At 1,200 years after abandonment, the permeability of the borehole below the waste panel is decreased by one order of magnitude as a result of salt creep.	Natural Borehole Fluid Flow (H31) Waste-Induced Borehole Flow (H32)	R
CRA-2004, Chapter 6.0, Section 6.4.7.2.3 The Three-Plug Configuration	BRAGFLO	In addition to the two-plug configuration, a third plug is placed within the Castile above the brine reservoir. The third plug is assumed not to fail over the regulatory time period.	Natural Borehole Fluid Flow (H31) Waste-Induced Borehole Flow (H32)	Reg.-R
CRA-2004 Section 6.4.8 Castile Brine Reservoir MASS-18.0 Castile Brine Reservoir	BRAGFLO	The Castile region is assigned a low permeability, which inhibits fluid flow. Brine occurrences in the Castile are bounded systems. Brine reservoirs under the waste panels are assumed to have limited extent and interconnectivity, with effective radii on the order of several hundred meters.	Brine Reservoirs (N2)	R
CRA-2004, Chapter 6.0, Section 6.4.9 Climate Change MASS-17.0 Climate Change	SECOTP2D	Climate-related factors are treated through recharge. A parameter called the Climate Index is used to scale the Culebra flux field.	Climate Change (N61) Temperature (N60) Precipitation (e.g., Rainfall) (N59)	R

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C = Conservative
Reg. - Based on regulatory guidance
1 See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.10 Initial and Boundary Conditions for Disposal System Modeling CRA-2004, Chapter 6.0, Section 6.4.10.1 Disposal System Flow and Transport Modeling (BRAGFLO and NUTS)	BRAGFLO	There are no gradients for flow in the far-field of the Salado, and pressures are above hydrostatic but below lithostatic. Excavation and waste emplacement result in partial drainage of the DRZ.	Saturated Groundwater Flow (N23) Brine Inflow (W40)	R
	BRAGFLO	An initial water-table surface is set in the Dewey Lake at an elevation of 980 meters (m) (3,215 feet [ft]) above mean sea level. The initial pressures in the Salado are extrapolated from a sampled pressure in MB139 at the shaft and are in hydrostatic equilibrium. The excavated region is assigned an initial pressure of one atmosphere. The liquid saturation of the waste-disposal region is consistent with the liquid saturation of emplaced waste. Other excavated regions are assigned zero liquid saturation, except the shaft, which is fully saturated.	Saturated Groundwater Flow (N23)	R
	NUTS	Molecular transport boundary conditions are no diffusion or dispersion in the normal direction across far-field boundaries. Initial An concentrations are zero everywhere, except in the waste.	Radionuclide Decay and Ingrowth (W12) Solute Transport (W77)	R
CRA-2004, Chapter 6.0, Section 6.4.10.2 Culebra Flow and Transport Modeling (MODFLOW-2000, SECOTP2D)	MODFLOW-2000	Constant head and no-flow boundary conditions are set on the far-field boundaries of the flow model.	Saturated Groundwater Flow (N23)	R
	MODFLOW-2000	Initial An concentrations in the Culebra are zero.	Solute Transport (W77)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.10.3 Initial and Boundary Conditions for Other Computational Models	NUTS PANEL BRAGFLO (DBR) CUTTINGS_S	Initial and boundary conditions interpolated from previously executed BRAGFLO calculation.	—	R
CRA-2004, Chapter 6.0, Section 6.4.12 Sequences of Future Events	CCDFGF	Each 10,000-year future (random sequence of future events) is generated by randomly and repeatedly sampling (1) the time between drilling events, (2) the location of drilling events, (3) the activity level of the waste penetrated by each drilling intrusion, (4) the plug configuration of the borehole, and (5) the penetration of a Castile brine reservoir, and by randomly sampling the occurrence of mining in the disposal system.	Oil and Gas Exploration (H1) Potash Exploration (H2) Oil and Gas Exploitation (H4) Other Resources (H8) Enhanced Oil and Gas Recovery (H9) Natural Borehole Fluid Flow (N31) Waste-Induced Borehole Flow (H32)	Reg.-R
CRA-2004, Chapter 6.0, Section 6.4.12.1 Active and Passive Institutional Controls in Performance Assessment Chapter 7.0	CCDFGF	Active institutional controls are effective for 100 years and completely eliminate the possibility of disruptive human activities (e.g., drilling and mining). No credit is taken for passive institutional controls.	—	Reg.-R
CRA-2004, Chapter 6.0, Section 6.4.12.2 Number and Time of Drilling Intrusions	CCDFGF	Drilling may occur after 100 years according to a Poisson process.	Loss of Records (H57) Oil and Gas Exploration (H1) Potash Exploration (H2) Oil and Gas Exploitation (H4) Other Resources (H8)	Reg.-R
CRA-2004, Chapter 6.0, Section 6.4.12.3 Location of Intrusion Boreholes	CCDFGF	The waste disposal region is discretized into 144 regions, each with an equal probability of being intersected. A borehole can penetrate only one region.	Disposal Geometry (W1)	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
CRA-2004, Chapter 6.0, Section 6.4.12.4 Activity of the Intersected Waste Appendix TRU WASTE	CCDFGF	Six-hundred ninety waste streams are identified as contact-handled (CH) transuranic (TRU) (CH-TRU). All 77 remote-handled (RH) transuranic (TRU) (RH-TRU) waste streams were grouped (binned) together into one equivalent or average (WIPP-scale) RH-TRU waste stream.	Heterogeneity of Waste Forms (W3)	R
CRA-2004, Chapter 6.0, Section 6.4.12.5 Diameter of the Intrusion Borehole CCA Appendix DEL	CUTTINGS_S	The diameter of the intrusion borehole is constant at 12.25 inches (in.) (31.12 centimeters [cm]).	—	Reg.-R
CRA-2004, Chapter 6.0, Section 6.4.12.6 Probability of Intersecting a Brine Reservoir	CCDFGF	One brine reservoir is assumed to exist below the waste panels. The probability that a deep borehole intersects a brine reservoir below the waste panels is sampled uniformly from 0.01 to 0.60.	Brine Reservoirs (N2)	R
CRA-2004, Chapter 6.0, Section 6.4.12.7 Plug Configuration in the Abandoned Intrusion Borehole	CCDFGF	The two-plug configuration has a probability of 0.696. The three-plug configuration has a probability of 0.289. The continuous concrete plug has a probability of 0.015.	—	Reg.-R
CRA-2004, Chapter 6.0, Section 6.4.12.8 Probability of Mining Occurring in the Land Withdrawal Area	CCDFGF	Mining in the disposal system occurs a maximum of once in 10,000 years (a 10^{-4} probability per year).	—	Reg.-R
CRA-2004, Chapter 6.0, Section 6.4.13 Construction of a Single Complementary Cumulative Distribution Function (CCDF)	CCDFGF	Deterministic calculations are executed with BRAGFLO, NUTS, MODFLOW-2000, SECOTP2D, CUTTINGS_S, and PANEL to generate reference conditions. These reference conditions are used to estimate the consequences associated with random sequences of future events. These are, in turn, used to develop CCDFs.	—	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	CCDFGF	Ten thousand random sequences of future events are generated for each CCDF plotted.	—	R
CRA-2004, Chapter 6.0, Section 6.4.13.1 Constructing Consequences of the Undisturbed Performance Scenario	CCDFGF	A BRAGFLO and NUTS calculation with undisturbed conditions is sufficient for estimating the consequences of the undisturbed performance scenario.	—	R
CRA-2004, Chapter 6.0, Section 6.4.13.2 Scaling Methodology for Disturbed Performance Scenarios	CCDFGF	Consequences for random sequences of future events are constructed by scaling the consequences associated with deterministic calculations (reference conditions) to other times, generally by interpolation, but sometimes by assuming either similarity or no consequence.	—	R
CRA-2004, Chapter 6.0, Section 6.4.13.3 Estimating Long-Term Releases from the E1 Scenario	CCDFGF NUTS	Reference conditions are calculated or estimated for intrusions at 100, 350, 1,000, 3,000, 5,000, 7,000, and 9,000 years.	Waste-Induced Borehole Flow (H32)	R
CRA-2004, Chapter 6.0, Section 6.4.13.4 Estimating Long-Term Releases from the E2 Scenario	CCDFGF NUTS SECOTP2D	The methodology is similar to the methodology for the E1 scenario. For multiple E1 intrusions into the same panel, the additional source term to the Culebra for the second and subsequent intrusions is assumed to be negligible.	Waste-Induced Borehole Flow (H32) Waste Inventory (W2)	R
CRA-2004, Chapter 6.0, Section 6.4.13.5 Estimating Long-Term Releases from the E1E2 Scenario	CCDFGF PANEL	The concentration of actinides in liquid moving up the borehole assumes homogeneous mixing within the panel.	Waste-Induced Borehole Flow (H32)	C
	PANEL	Any actinides that enter the borehole for long-term flow calculations reach the Culebra.	Waste-Induced Borehole Flow (H32)	C

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

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Table MASS-5. General Modeling Assumptions (Continued)

Chapter or Section	Code	Modeling Assumption	Related FEP in Appendix SCR-2009	Assumption Considered[a]
	CCDFGF PANEL	Reference conditions are calculated or estimated for intrusion at 100, 300, 1,000, 2,000, 4,000, 6,000 and 9,000 years.	Oil and Gas Exploration (H1)	—
CRA-2004, Chapter 6.0, Section 6.4.13.6 Multiple Scenario Occurrences	CCDFGF PANEL	The panels are assumed not to be interconnected for long-term brine flow.	Saturated Groundwater Flow (N23) Unsaturated Groundwater Flow (N24)	R
CRA-2004, Chapter 6.0, Section 6.4.13.7 Estimating Releases During Drilling for All Scenarios	CCDFGF PANEL NUTS	Repository conditions will be dominated by Castile brine if any borehole connects to a brine reservoir.	Brine Reservoirs (N2) Natural Borehole Fluid Flow (H31)	R
	CUTTINGS_S PANEL CCDFGF	Depletion of actinides in parts of the repository penetrated by boreholes is not accounted for in calculating the releases from subsequent intrusions at such locations.	Waste-Induced Borehole Flow (H32) Waste Inventory (W2)	C
CRA-2004, Chapter 6.0, Section 6.4.13.8 Estimating Releases in the Culebra and the Impact of the Mining Scenario	CCDFGF	Releases from intrusions at random times in the future are scaled from releases calculated at 100 years with a unit source of radionuclides in the Culebra.	—	R
	CCDFGF	Actinides in transit in the Culebra when mining occurs are transported in the flow field used for the undisturbed case. Actinides introduced subsequent to mining are transported in the flow field used for the disturbed case (i.e., the mined case).	—	R

[a] R = Reasonable
C = Conservative
Reg. - Based on regulatory guidance
See above - Refers to assumptions 1 through 8 listed at the beginning of this table.

necessarily zero. This effect, which results in additional flux of gas above that predicted by application of Darcy's Law, is known as the slip phenomenon, or Klinkenberg effect (Bear 1972, p. 128). A correction to Darcy's Law for the Klinkenberg effect is incorporated into the BRAGFLO model (see Appendix PA-2009, Section PA-4.2).

Darcy flow for one and two phases implies that values for principal fluid and rock parameters must be specified. Fluid properties in the Darcy flow model used for the WIPP PA are density, viscosity, and compressibility, while rock properties are porosity, permeability, and

compressibility (pore or bulk). In BRAGFLO, other parameters are required to describe the interactions or interference between the gas and brine phases present in the model because those phases can occupy the same pore space. In the WIPP application of Darcy flow models, compressibility of both the liquid and rock are related to porosity through a dependence on pressure. Fluid density, viscosity, and compressibility are functions of fluid composition, pressure, and temperature. It is assumed in BRAGFLO that fluid viscosity is a function of pressure, but its density and compressibility are held constant. Fluid composition for the purposes of modeling flow and transport is assumed to be constant.

MASS-3.2 Hydrogen Gas as Surrogate for Waste-Generated Gas Physical Properties in BRAGFLO and DRSPALL

Hydrogen gas is produced as a result of the corrosion of steel in the repository by water or brine. As in the CCA, the gas phase in the BRAGFLO model is assigned the properties of hydrogen because hydrogen will, under most conditions reasonable for the WIPP, be the dominant component of the gas phase. The model for spallings, DRSPALL, also assigns the physical properties of hydrogen to the gas phase. As discussed in the following text, the effect of assuming flow of pure H_2 instead of a mixture of gases (including H_2, CO_2, H_2S, and CH_4), was shown to be minor relative to the permeability variations in the surrounding formations.

Other gases may be produced by processes occurring in the repository. If microbial degradation occurs, a significant amount of CO_2 and possibly methane (CH_4) will be generated by microbial degradation of cellulosics and, possibly, plastics and rubbers in the waste. The CO_2 produced, however, will react with the magnesium-oxide (MgO) engineered barrier and cementitious materials to form brucite ($Mg(OH)_2$), hydromagnesite ($Mg_5(CO_3)_4(OH)_2{\cdot}4H_2O$), and calcite ($CaCO_3$) thus resulting in very low CO_2 fugacity in the repository. Although other gases exist in the disposal system, BRAGFLO calculations assume these gases are insignificant and they are not included in the model.

With the average stoichiometry gas generation model, the total number of moles of gas generated will be the same whether the gas is considered to be pure H_2 or a mixture of several gases, because the generation of other gases is accounted for by specifying the stoichiometric factor y (see Appendix PA-2009, Section PA-4.2.5). Therefore, considering only the moles of gas generated, the pressure buildup in the repository will be approximately the same because the expected gases behave similarly to an ideal gas, even up to lithostatic pressures.

The effect of assuming pure H_2 instead of a mixture of gases (including H_2, CO_2, H_2S and CH_4) on flow behavior, and its resulting impact on the WIPP repository pressure, is as follows:

Radial flow in a fully saturated rock with nonideal gas is described by Darcy's Law, which, for the given problem, has a solution of the form (Amyx, Bass, and Whiting 1960, p. 78, Equation 2-33)

$$q_b = 1.988\times10^{-5}\left[\frac{T_b Z_b}{P_b}\frac{kh\left(P_e^2 - P_w^2\right)}{\mu_{avg} Z_{avg}\ln\left(\frac{r_e}{r_w}\right)}\right] \quad \text{(MASS.1)}$$

which can be rewritten as

$$P_e^2 - P_w^2 = \frac{q_b P_b}{1.988\times10^{-5} T_b Z_b}\times\frac{\mu_{avg} Z_{avg}}{kh}\ln\left(\frac{r_e}{r_w}\right) \quad \text{(MASS.2)}$$

where

- q = gas flow rate (cubic feet per day at base (reference) conditions)
- T = temperature (K)
- P = pressure (pounds per square inch absolute)
- k = permeability (millidarcys)
- h = height (feet)
- μ = viscosity (centipoises)
- Z = gas compressibility factor (defined as the ratio of the actual molar volume of a gas to the corresponding ideal gas volume *RT/P* at the same temperature and pressure)
- r = radius (consistent units)
- R = ideal gas constant
- e = denotes external boundary (repository)
- w = denotes internal boundary (wellbore)
- b = denotes base or reference conditions for gas (temperature, pressure, compressibility factor)
- avg = denotes average properties between external and internal boundaries because u and z are functions of pressure which change with time

This expression is useful for examining the effects of gas properties, specifically the viscosity (μ) and the compressibility (Z) and rock properties (namely k), on the flow rate (q) and the pressure (P).

To evaluate the effect of gas composition on q and P, SUPERTRAPP, a computer program developed by the National Institute of Standards and Technology (NIST), was used (National Institute of Standards and Technology 1992). SUPERTRAPP calculates gas properties for 116 pure fluids and mixtures of up to 20 components for temperatures to 1,000 K (726 °C, 1340 °F) and pressures to 300 megapascals (MPa). Because such small quantities of H_2S are anticipated at the WIPP, its impact is negligible.

Figure MASS-1 shows the relationship between gas viscosity and composition of H_2-CO_2 mixtures for various mole fractions of H_2 at pressures of 7 MPa and 15 MPa, as determined from SUPERTRAPP. The viscosity at 50% mole fraction H_2 is about 2.3 times greater than for 100% mole fraction H_2. As shown in Equation (MASS.1), viscosity has an inverse relationship to flow rate and, as shown in Equation (MASS.2), a direct relationship to the square of the repository

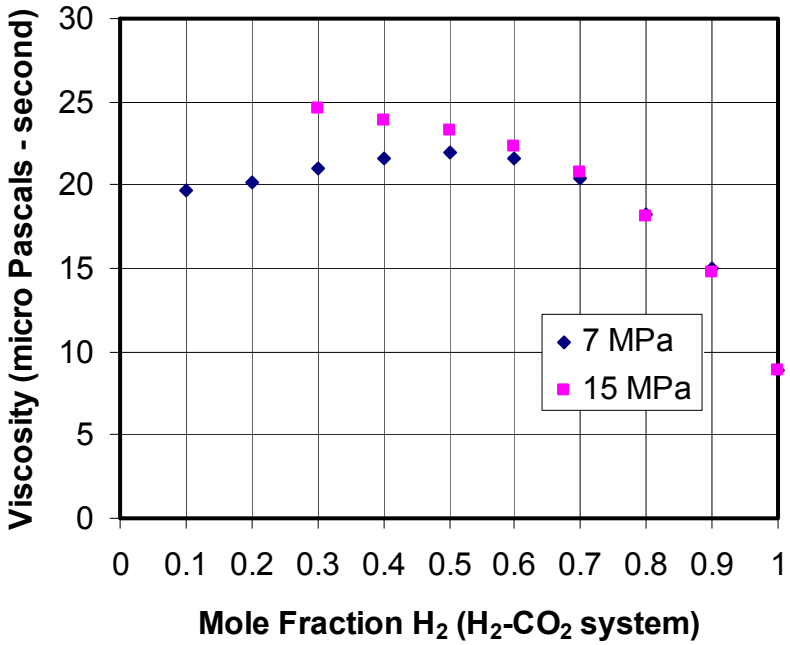


Figure MASS-1. Gas Viscosity as a Function of Mole Fraction H_2 at 7 MPa and 15 MPa Pressure

pressure. Hence, viscosity differences that would result if gas properties other than those of hydrogen were incorporated would result in a decrease in flow rate and potentially higher pressures.

As shown in Figure MASS-2, the gas compressibility at 50% mole fraction H_2 is about 0.9 times that of pure H_2. Like viscosity, the gas compressibility (actual volume/ideal volume) is inversely related to flow rate and directly related to the square of the repository pressure. Therefore, the impact of variation in gas compressibility caused by composition is considered minor and is not considered.

The viscosity and compressibility calculations described above for H_2-CO_2 mixtures were repeated for H_2-CH_4 mixtures for various mole fractions of H_2 at pressures of 7 MPa and 15 MPa (Kanney 2003). The variability of viscosity with the composition for the H_2-CH_4 mixtures is smaller than that observed for the H_2-CO_2 mixtures. For example, at 15 Mpa, the gas viscosity of H_2-CH_4 at 50% mole fraction is only 1.6 times greater than the viscosity at 100% mole fraction. The H_2-CH_4 mixtures are only slightly less compressible than the H_2-CO_2 mixtures. For example, at 15 MPa, the gas compressibility of the H_2-CH_4 at 50% mole fraction is approximately 0.94 times the compressibility at 100% mole fraction. Changing composition from 100% to 50% H_2 would result in a slight increase in flow rate and a decrease in pressure.

The permeability of each component of the formation plays a significant role in determining both flow rate and pressure. Because marker bed (MB) permeabilities and Salado impure halite permeabilities vary over three to four orders of magnitude (see Fox 2008, Table 30 and Table 31), the permeabilities of these flow pathways will have a greater influence on pressure and flow rate determinations than either uncertainty in viscosity or gas compressibility effects.

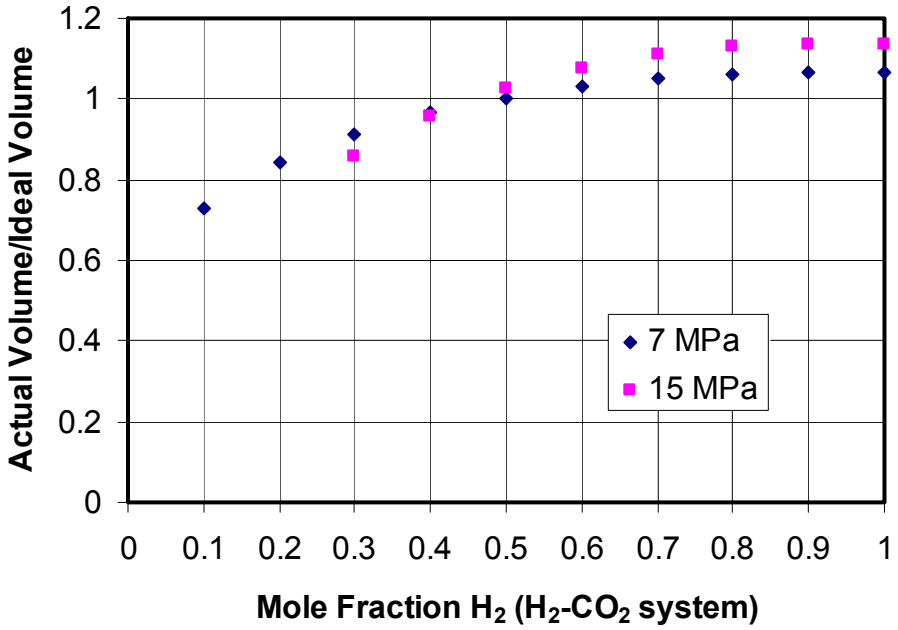


Figure MASS-2. Gas Compressibility as a Function of Mole Fraction H_2

Note that the BRAGFLO code includes a pressure-induced fracture model that will limit pressure increases in the repository (Schreiber 1997). For example, at high repository pressures, the factor of 1.5 pressure increase calculated here using the simplified Darcy's Law model is unlikely to be seen in the BRAGFLO results, since fracturing will lead to increased permeability, effectively limiting pressure increases.

MASS-3.3 Salado Brine as Surrogate for Liquid-Phase Physical Properties in BRAGFLO

BRAGFLO uses Salado Formation brine properties as the physical properties for all liquids. However, liquid in the modeled region may consist of (1) brine originally in the Salado, (2) liquid introduced in the excavation during construction, maintenance, and ventilation during the operational phase, (3) a very small amount of liquid introduced as a component of the waste, (4) liquid from overlying units, and (5) liquid from the Castile brine reservoir. However, for BRAGFLO modeling, it is assumed that the properties of all of these liquids are similar enough to Salado brine properties that the effect of any variation in properties resulting from liquids mixing is negligible. The variations in chemical properties of brine are accounted for as discussed in Appendix SOTERM-2009, Section SOTERM-2.0, Section SOTERM-2.3, and Section SOTERM-5.0.

MASS-4.0 Model Geometries

This section presents supplementary information on the disposal system geometry.

MASS-4.1 Disposal System Geometry as Modeled in BRAGFLO

Overall, the conceptual model of the disposal system geometry represents the spatial effects of process interactions in two dimensions. The geometry used to represent long-term fluid flow processes in the Salado, flow between a borehole and overlying units and flow within the repository (where processes coupled to fluid flow such as creep closure and gas generation occur), is a vertical cross-section through the repository on a north-south axis shown in Figure MASS-3 (see also Appendix PA-2009, Section PA-4.2.1). The dimension of this geometry in the direction perpendicular to the plane of the cross-section varies so that spatial effects of certain processes can be better represented.

For fluid flow and transport modeling in the Culebra, the geometry is a horizontal, two-dimensional plane (see Appendix PA-2009, Section PA-4.8, Figure PA-32). For modeling brine flow from the intruded panel to the borehole during drilling (DBR), the geometry is a two-dimensional, horizontal representation of a waste panel as described in Section MASS-16.2 (see also the CRA-2004, Chapter 6.0, Section 6.4.7.1).

Using a two-dimensional geometry to represent the three-dimensional Salado flow is based on the assumption that brine and gas flow will converge upon and diverge from the repository horizon. Grid flaring is used when flows can be represented as divergent and convergent from the center of the flaring (see Section MASS-4.2.5). The impact of this conceptual model and its implementation in a two-dimensional grid has been compared to a model that does not make the assumption of convergent and divergent flow (see the CRA-2004, Appendix PA, Attachment MASS, Attachment 4-1 for additional information). The conceptual model for the Salado also includes the slight and variable dip of beds in the vicinity of the repository, which might affect fluid flow.

Above and below the repository, it is assumed that any flow between the borehole or shaft (see the CRA-2004, Chapter 6.0, Section 6.4.3) and surrounding materials will converge or diverge. With respect to flow in units overlying the Salado, the only purpose of this conceptual model is to determine the quantity (flux) of fluid leaving or entering the borehole or shaft. Fluid movement through the units above the Salado is treated in a different conceptual model (see the CRA-2004, Chapter 6.0, Section 6.4.6). Below the repository, the possible presence of a brine reservoir is considered to be important, so a hydrostratigraphic layer representing the Castile and a possible brine reservoir in it is included (see the CCA, Appendix MASS, Section MASS-4.2 for the disposal system geometry historical context prior to the CCA).

MASS-4.2 Change to Disposal System Geometry since the CCA

Changes have been made to the disposal system geometry since the first WIPP certification. The disposal system geometry is specifically represented in BRAGFLO. This section describes the methodology used to create the two-dimensional BRAGFLO computational grid used for the

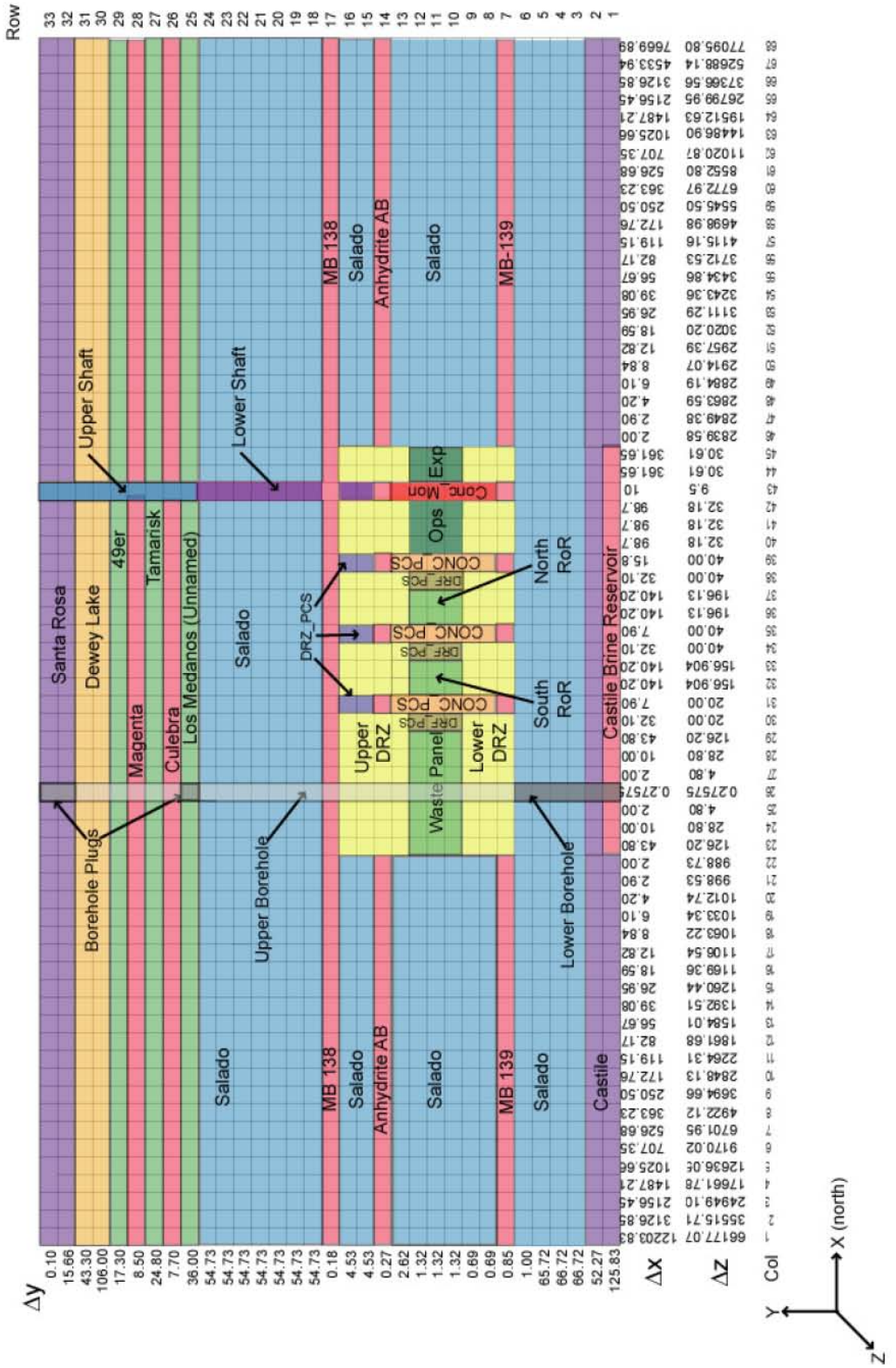


Figure MASS-3. Logical Grid Used for the CRA-2004 and 2009 PA BRAGFLO Calculations

CRA-2004 PA calculations. The CRA-2004 grid is similar to the CCA and the CCA Performance Assessment Verification Test (PAVT) grids, except for the differences described below. Since no changes have been made to the geometry since the CRA-2004 PABC, this grid was used in the CRA-2009 PA.

The most important changes affecting the CRA-2004 BRAGFLO grid were the implementation of the Option D panel closures and a simplified shaft seal model. Additional grid refinements were also made to increase numerical accuracy and computational efficiency and to reduce numerical dispersion. These changes modify the conceptual models. All conceptual model changes were approved by the Salado Flow Peer Review Panel in February 2003 (Caporuscio, Gibbons, and Oswald 2003). For completeness, all changes from the CCA PA/CCA PAVT grid are described here. These changes were made and approved by the EPA in the 2004 recertification decision (U.S. Environmental Protection Agency 2006) and are repeated here for completeness and to show the historical progression of the grid from the CCA to the CRA-2009 PA.

MASS-4.2.1 CCA to CRA-2004 Baseline Grid Changes

The baseline grid used in the CCA PA and the CCA PAVT had 33 cells in the x direction and 31 cells in the y direction, while the grid used for the CRA-2004 PA and later calculations has dimensions 68 by 33 cells. The specific changes implemented in the CRA-2004 grid are listed below and discussed in more detail in the following sections. Logical grids for the CCA PA, the CCA PAVT, and the CRA-2004 and CRA-2009 PAs are shown in Figure MASS-3 and Figure MASS-4.

The following changes have been implemented in the CRA-2004 grid:

1. A simplified shaft seal model is implemented.
2. Option D-type panel closures are implemented.
3. Segmentation of the waste regions is increased.
4. A grid-flaring method is redefined and simplified.
5. X spacing of the grid beyond the repository to the north and south is refined.
6. Layers above and below MB 139 have been made relatively thin (~1 m thick), and Y spacing in the Salado has been changed.

MASS-4.2.2 CRA-2004 Simplified Shaft Seal Model

A shaft seal model is included in the CRA-2004 grid, but it is implemented in a simpler fashion than that used for the CCA PA and the CCA PAVT. A detailed description of the parameters used to define the simplified model is discussed in AP-094 (James and Stein 2002) and the resulting analysis report (James and Stein 2003). The model used in the CRA-2004 PA is described by Stein and Zelinski (2003a and 2003b), and was approved by the Salado Flow Peer Review Panel (Caporuscio, Gibbons, and Oswald 2003).

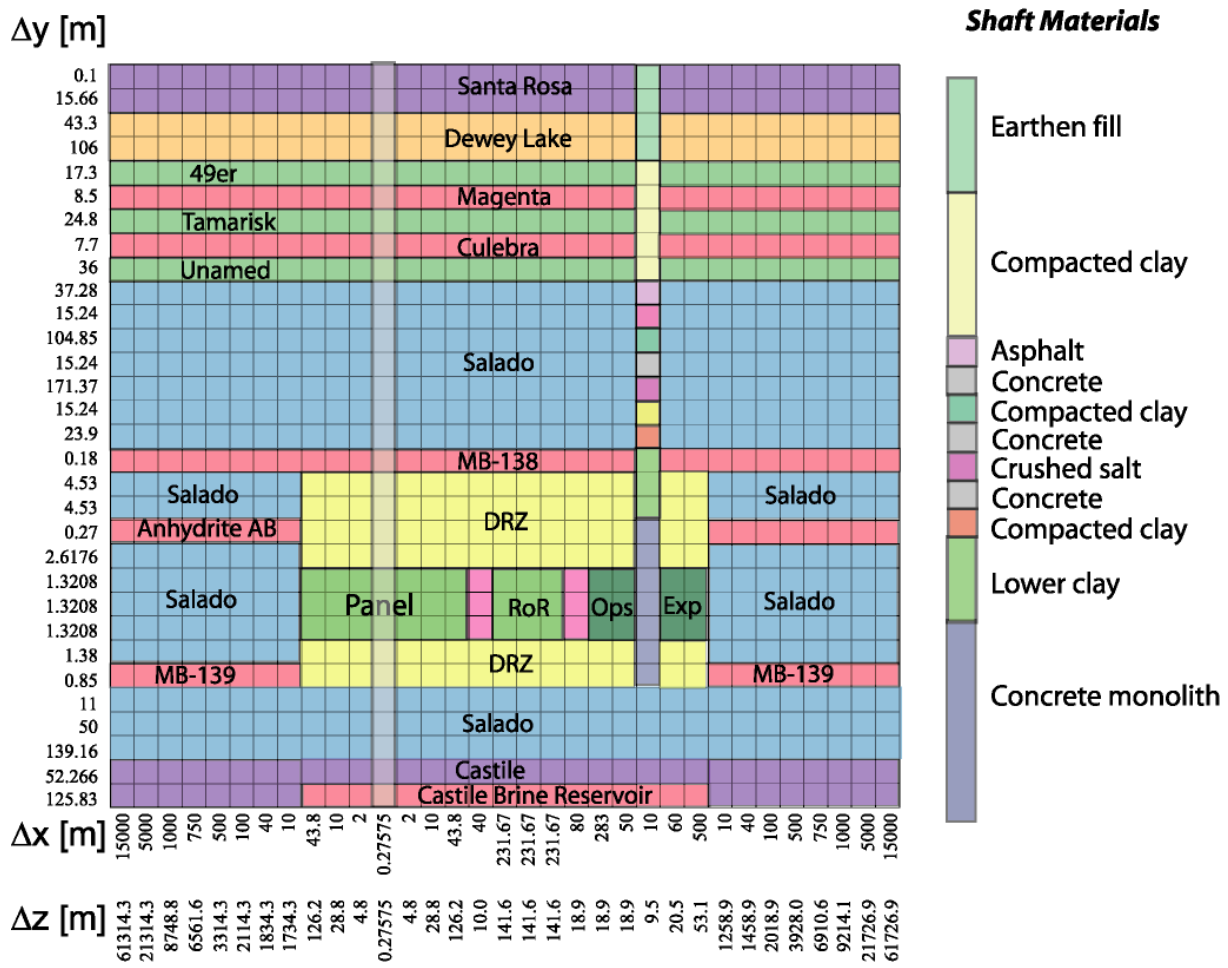


Figure MASS-4. Logical Grid Used for the CCA PA BRAGFLO Calculations

The new model does not alter the conceptual model of the shaft seal components as described in the CCA. Rather, it simplifies the representation of seal components in the repository system model. The CRA and CCA shaft models are graphically compared in Figure MASS-5. The simplified shaft model was tested in the AP-106 calculations (Stein and Zelinski 2003a and 2003b), which supported the Salado Flow Peer Review (see the CRA-2004, Chapter 9.0, Section 9.1.3.4). The results of this analysis demonstrated that brine flow through the simplified shaft model was comparable to brine flows through the detailed shaft model in the CCA PAVT calculations. The conclusion remains that the shaft seals are very effective barriers to flow throughout the 10,000-year regulatory period. The CRA-2004 PA shaft representation is used in the CRA-2009 PA.

MASS-4.2.3 CRA-2004 Implementation of Option D-Type Panel Closure

In the CCA, the DOE presented four options for panel closure designs (A through D). Upon reviewing the CCA, the EPA mandated the implementation of the Option D design. For the

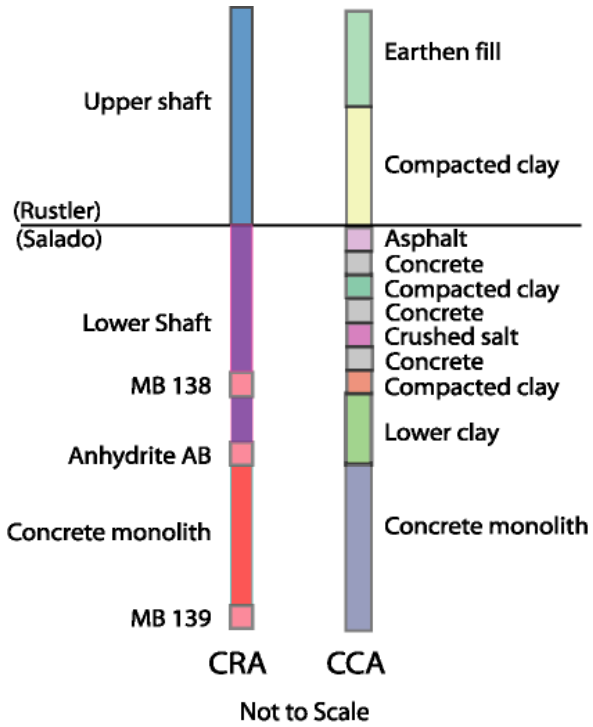


Figure MASS-5. Comparison of the Simplified Shaft (CRA-2004 and CRA-2009) and the Detailed Shaft (CCA) Models

CRA-2004, the true cross-sectional area of the Option D panel closures was represented in the flow model. In addition, to appropriately represent the effect of Option D geometry on repository fluid flow, the segmentation of the waste regions was increased in the grid. This change is described fully in the CRA-2004, Appendix PA, Attachment MASS, Section MASS-4.2.4. The CRA-2009 PA continues to use the same panel closure representation as the CRA-2004 PA.

For CRA-2004, three sets of panel closures are included in the model domain. The southernmost set of closures represents a pair of closures separating a single waste panel from the other waste areas. The middle set of closures represents four panel closures that will be emplaced between the southern and northern extended panels. The northernmost set of panel closures represents two sets of four panel closures that will be emplaced between the waste regions and the shaft seals.

Each set of panel closures is represented in the CRA-2004 grid with four materials. Refer to Figure MASS-6.

1. CONC_PCS: This material represents the concrete monolith, which has properties of Salado Mass Concrete (SMC).

2. DRZ_PCS: This material represents the DRZ immediately above the concrete monolith that is expected to heal after the emplacement of the monolith.

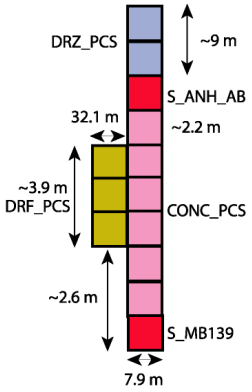


Figure MASS-6. Logical Grid Representation of the Option D Panel Closures for the CRA

3. DRF_PCS: This material represents the empty drift and explosion wall portion of the panel closure. This material has the same properties as WAS_AREA (including creep closure).

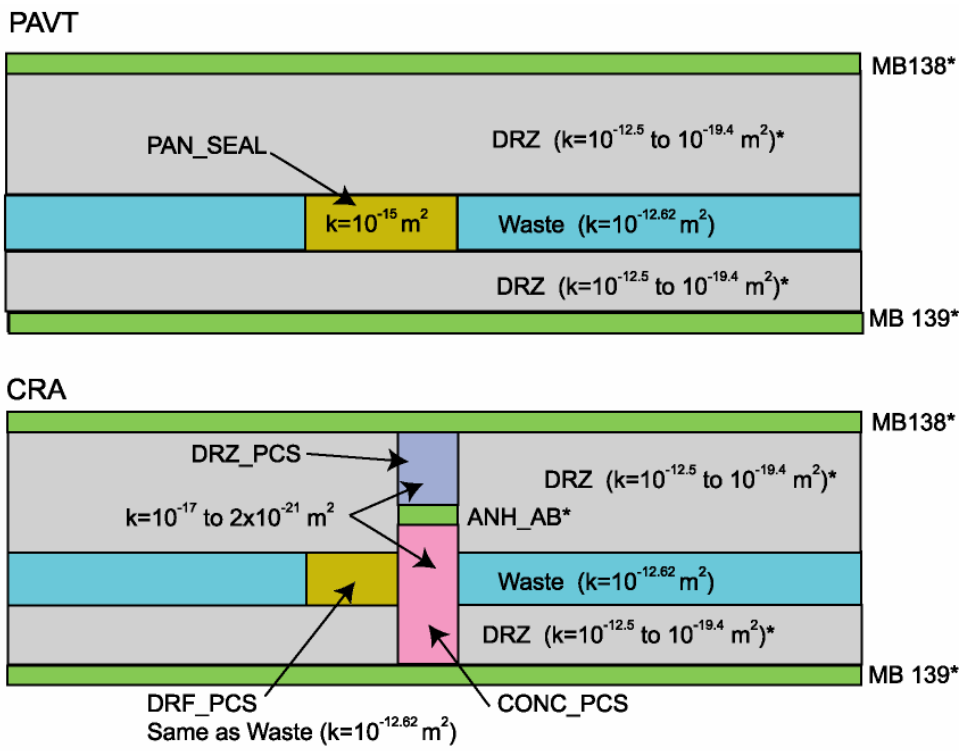
4. MB materials S_ANH_AB and S_MB 139: These materials are the same as those used to represent the anhydrite MBs in other parts of the grid. MB materials were used because they have permeability ranges very close to the material CONC_PCS and in the case when pressures near the panel closures exceed the fracture initiation pressure of the MBs, fractures could extend around the concrete monolith out of the 2-D plane represented by the numerical grid. By using MB materials to represent the parts of the panel closures that intersect MBs, both the permeability of the closure and the potential fracture behavior of MB material near the closures are represented.

Figure MASS-7 is a schematic diagram comparing the panel closure implementation in the CCA and CRA-2004 grids. Permeability ranges are indicated for all materials. Figure MASS-6 shows the 13 grid cells used to represent each set of Option D panel closures in the CRA-2004 BRAGFLO grid.

MASS-4.2.4 Increased Segmentation of Waste Regions in Grid

The CCA PA/CCA PAVT grid divided the waste region into two regions: a single panel in the southern end of the repository referred to as the Waste Panel, and a larger region containing the other nine panels referred to as the RoR. The Waste Panel is intersected by an intrusion borehole and is used to represent conditions in any panel intersected by a borehole.

It is assumed that the Option D panel closures are effective at impeding flow between panels. Therefore, it was considered necessary to divide the rest of repository (RoR) into northern and southern blocks separated by a set of panel closures. The south RoR block represents conditions in a panel directly adjacent to an intruded panel. The north RoR block represents conditions in a nonadjacent panel far from the intruded panel (i.e., it has at least two panel closures between it and the intruded panel). This representation assumes that the effects of drilling intrusions will be damped in nonintruded panels, and the degree of damping will depend on the proximity of the drilling intrusion and the number of panel closures separating the intruded panel from other regions of the repository. The CRA-2009 PA uses the same segmentation of the waste regions as in the CRA-2004 PA. (See the CRA-2004, Appendix PA, Attachment MASS, Section MASS-4.2.4 for a description of waste-region segmentation.)



[* = allowed to fracture, permeability is pressure dependant above ~12.5 MPa]

Figure MASS-7. Schematic Comparison of the Representation of Panel Closures in the CCA PAVT and CRA-2004

MASS-4.2.5 CRA-2004 Redefined and Simplified Grid Flaring Method

Grid flaring is a method to represent three-dimensional volumes in a two-dimensional grid. Flaring is used when flows can be represented as divergent and convergent from the center of flaring. The CCA PA/CCA PAVT grid used flaring at two different scales: locally around the borehole and shaft, and regionally to the north and south of the excavated regions (around a point in the northern end of the RoR). For the CRA-2004 PA, the local flaring around the borehole is the same as in the CCA PA/CCA PAVT grid. The local flaring around the shaft was eliminated because it had been demonstrated not to be a release pathway. Likewise, the manner in which the regional flaring was calculated has been simplified. The CRA-2009 PA uses the same grid flaring as in the CRA-2004 PA. (See the CRA-2004, Appendix PA, Attachment MASS, Section MASS-4.2.5 for a description of grid flaring).

MASS-4.2.6 CRA-2004 Refinement of the X-Spacing Outside the Repository

The grid blocks to the north and south of the excavated region were refined in the x-direction from the baseline grid. The x dimension of the grid cells immediately to the north and south of the repository starts at 2 m and increases by a factor of 1.45.

Exceptions to this are made to ensure that the location of the Land Withdrawal Boundary and the total extent of the grid matches that in the baseline grid. This CRA-2004 PA refinement factor was chosen to reduce numerical dispersion caused by rapid increases in cell dimensions (Anderson and Woessner 1992 and Wang and Anderson 1982). The CRA-2009 PA continues to use this refinement.

MASS-4.2.7 CRA-2004 Refinement of the Y-Spacing

During the CRA-2004 PA, the y direction grid spacing within the layers representing the Salado was changed from the CCA PA/CCA PAVT grid spacing. The Salado grid spacing used in the CCA PA was dictated by the thickness of different shaft seal materials. Since the shaft is no longer represented in the model domain, the y spacing in the Salado is now uniform. In addition, two layers were added immediately above and below MB 139 to refine the grid spacing and reduce numerical dispersion. These changes resulted in a total of 33 y divisions for the grid, and increased the numerical accuracy of flow and transport calculations.

The x and y direction refinements used in the CRA-2004 PA grid are included in the CRA-2009 PA.

MASS-5.0 BRAGFLO Geometry of the Repository

The BRAGFLO code uses a grid to represent the conceptual model of the repository geometry (see Figure MASS-3). As with the geometry of the disposal system discussed in the CRA-2004, Chapter 6.0, Section 6.4.2.1 and earlier in this appendix, the principal process considered in setting up the repository geometry is fluid flow. Several features considered to be important in fluid flow are included in the conceptual model. The first is the overall dimension of the repository along the north-south trend of the cross section, as well as the major divisions within the repository (i.e., waste disposal region, operations region, and experimental region). The second is the volume of a single panel, because fluid flow to a borehole penetrating the repository may have direct access only to the volume in a waste panel. Access to other regions of the repository may require flow through or around a panel closure. The third feature is the physical dimensions of panel closures separating the single panel and the other major divisions of the repository.

Notably absent from the conceptual model for the long-term performance of the repository are pillars and individual drifts and rooms. These are excluded from the model for simplicity, and it is assumed that they have either negligible impact on fluid-flow processes or, alternatively, that including them in the conceptual model would be beneficial to long-term performance because their presence could make flow paths more tortuous and decrease fluxes. This assumption includes lumping four and five of the 10 panels into the south RoR and north RoR regions respectively (see the CRA-2004, Appendix PA, Attachment MASS, Section MASS-4.2.4).

The BRAGFLO model of the WIPP disposal system is a two-dimensional array of three-dimensional grid blocks. Each grid block has a finite length, width, height, volume, and surface area for its boundaries with neighboring grid blocks. The BRAGFLO two-dimensional grid is similar to any other two-dimensional grid used to treat flows, except that the grid-block dimension in the z direction (perpendicular to the plane of the grid) varies from block to block as a function of the x direction (the lateral direction) (see the CRA-2004, Appendix MASS, Section MASS-4.2.5). This allows the BRAGFLO grid to treat important geometric aspects of the WIPP disposal system, such as the very small intrusion borehole, the moderate-sized shaft, and the larger controlled areas. The grid configurations used in the CCA PA and the CCA PAVT are shown in Figure MASS-4, while the grid used for the CRA-2004 PA and the CRA-2009 PA is shown in Figure MASS-3.

MASS-5.1 Historical Context of the Repository Model

Several early models of repository fluid-flow behavior—including models of radionuclide migration pathways, gas flow from the disposal area to the shaft, Salado brine flow through panel to borehole, effects of anhydrite layers on Salado brine flow through a panel, and flow from a brine reservoir through a disposal room—are summarized in Rechard et al. (1990, pp. 153–60). In the preliminary PA of 1992, all waste was lumped into a single region (WIPP Performance Assessment 1993). Because human intrusion boreholes were treated in detail for the CCA PA, it was necessary to model a single waste panel with a borehole surrounded by two-dimensional radial-flaring gridblocks. This approach is continued for the CRA-2009 PA. The CCA PA treated the remainder of the waste area as a single RoR. For the CRA-2004 PA and subsequent analyses, the RoR is divided into two areas separated by a panel closure system. As

discussed earlier, this change was made to more adequately simulate the effects of the Option D closure in impeding fluid flow between panels.

MASS-5.2 CRA-2009 Repository Model

The repository model for the CRA-2009 PA is the same model used in the CRA-2004 PABC. That model used the same features described for the CRA-2004 PA, with no changes to the representation of the repository geometry or BRAGFLO grid.

MASS-6.0 Creep Closure

The creep closure model used in the CRA-2009 is the same used in the CRA-2004 and the CRA-2004 PABC. The model used for creep closure of the repository is discussed in Appendix PORSURF-2009. Historical information on creep closure modeling is also contained in Appendix PORSURF-2009.

MASS-7.0 Repository Fluid Flow

Most repository fluid flow assumptions have not changed from those used in the CRA-2004 PABC. Those that did not change are discussed in Section MASS-7.1 and Section MASS-7.2 while those that did change are discussed in Section MASS-7.3. This model represents the long-term flow behavior of liquid and gas in the repository and its interaction with other regions in which fluid flow may occur, such as the Salado, shafts, or an intrusion borehole. This model is not used to represent the interaction of fluids in the repository with a borehole during drilling. Historical information on alternative conceptual models for brine inflow to the repository is contained in the CCA, Appendix MASS, Section MASS-7.0).

The first principle in the conceptual model for fluid flow in the repository is that gas and brine can both be present and mobile (two-phase flow), governed by conservation of energy and mass and by Darcy's Law for their fluxes (see Appendix PA-2009, Section PA-4.2). Consistent with typical concepts of two-phase flow, the phases can affect each other by impeding flow caused by partial saturation (relative permeability effects) and by affecting pressure caused by capillary forces (capillary pressure effects).

The flow of brine and gas in the repository is assumed to behave as two-phase, immiscible, Darcy flow (see Appendix PA-2009, Section PA-4.2). BRAGFLO is used to simulate brine and gas flow in the repository and to incorporate the effects of disposal-room closure and gas generation. Fluid flow in the repository is affected by the following factors:

- The geometric association of pillars, rooms, and drifts; panel closure caused by creep; and possible borehole locations
- The varied properties of the waste areas resulting from creep closure and heterogeneous contents
- Flow interactions with other parts of the disposal system
- Reactions that generate gas

The geometry of the panel around the intrusion borehole is consistent with the assumption that the fluid flow there will occur directly toward or directly away from the borehole. The geometry represents a semicircular volume north of the borehole and a semicircular volume south of the borehole (representing radial flow in a subregion of a two-dimensional representation of the repository).

Approximating convergent and divergent flow around the intrusion borehole creates a narrow neck in the otherwise fairly uniform width grid in the region representing the repository. In the undisturbed performance scenario, and under certain conditions in other scenarios, flow in the repository may pass laterally through this neck. In reality, this neck does not exist. Its presence in the model is expected to have a negligible or conservative impact on model predictions compared to predictions that would result from a more realistic model geometry. The time scale involved and the permeability contrast between the repository and surrounding rock are sufficient so that the lateral flow that may occur in the repository is restricted by the rate at which

liquid gets into or out of the repository, rather than by the rate at which it flows through the repository.

Gas generation is affected by the quantity of liquid in contact with metal. However, the distribution of fluid in the repository can only be approximated. For example, capillary action can create wicking that would increase the overall region in which gas generation occurs, but modeling this at the necessary resolution to simulate these processes would greatly increase the time required to carry out the modeling (Appendix PA-2009, Section PA-4.2.6 and CRA-2004, Section 6.4.3.3). Therefore, as a bounding measure for gas generation purposes, brine in the repository is distributed to an extent greater than estimated by the Darcy flow models or by the values of parameters chosen.

Option D panel closures and the surrounding rocks are represented by a group of materials, including

1. SMC
2. A material representing the empty drift and explosion wall
3. A material representing healed DRZ
4. MBs

SMC and healed DRZ materials are assigned permeability values sampled independently from a distribution ranging from 2×10^{-21} to 1×10^{-17} m^2. This value range is considered reasonable because the shape of the Option D closure assumes a compressive state that maintains a concrete permeability range similar to the CCA PAVT permeability. This range captures the uncertainty in the long-term performance of the Option D panel closure design.

Modeling of flow within the repository is based on homogenizing the room contents into relatively large computational volumes. The approach ignores heterogeneities in disposal room contents that may influence gas and brine behavior by causing fluid flow among channels or creating preferential paths in the waste, bypassing entire regions. Isolated regions could exist for several reasons:

- They may be isolated by low-permeability regions of waste that serve as barriers.
- Connectivity with the interbeds may occur only at particular locations within the repository.
- The repository dip may promote preferential gas flow in the upper regions of the waste.

For the CCA, the adequacy of the repository homogeneity assumption was examined in screening analyses DR-1 (Webb 1995) and DR-6 (Vaughn, Lord, and MacKinnon 1995a). These analyses used an additional parameter in BRAGFLO to specify the minimum active (mobile) brine flow saturation (pseudoresidual brine saturation). Above this saturation, the normal descriptions of two-phase flow apply (i.e., either the Brooks and Corey or van Genuchten and Parker relative permeability models). Below this minimum, brine is immobile, although it is available for reaction and may still be consumed during gas-generation reactions. The

assumption of a minimum saturation limit was justified based on the presumed heterogeneity of the waste and the slight dip in the repository. The minimum active brine saturation was treated as an uncertain parameter and sampled uniformly between the values 0.1 and 0.8 during the analysis. This saturation limit was applied uniformly throughout the disposal room to bound the impact of heterogeneities on flow (Webb 1995 and Vaughn, Lord, and MacKinnon 1995a). Results of this analysis showed that releases to the accessible environment in the baseline case (homogenization) are consistently higher.

The experimental and operations regions were represented in the CCA PA by a fixed porosity of 18.0% and a permeability of 10^{-11} m^2. The combination of low porosity and high permeability conservatively overestimated fluid flow through these regions and limited the capacity of these regions to store fluids, potentially overestimating releases to the environment. This conclusion was based on a screening analysis (Vaughn, Lord, and MacKinnon 1995b) that examined the importance of permeability varying with porosity in closure regions (waste disposal region, experimental region, and operations region). To perform this analysis, a model for estimating the change in permeability with porosity in the closure regions was implemented in BRAGFLO. A series of BRAGFLO simulations was performed to determine whether permeability varying with porosity in the closure regions could enhance contaminant migration to the accessible environment. Two basic scenarios were considered in the screening analysis: undisturbed performance and disturbed performance. To assess the sensitivity of system performance on dynamic permeability in the closure regions, CCDFs of normalized contaminated brine releases were constructed and compared with the corresponding baseline conditional CCDFs. The baseline model treated permeabilities in the closure regions as fixed values. Results of this analysis showed that the inclusion of dynamic closure of the waste disposal region, experimental region, and operations region in BRAGFLO resulted in computed releases to the accessible environment that are essentially equivalent to the baseline case.

A separate analysis (Park and Hansen 2003) examined the possible effects of heterogeneity in waste container and waste material strength on room closure. The analysis of room closure found that the room porosity may vary widely depending on the type of waste container and the emplacement of waste in the repository. However, analysis of a separate PA (Hansen et al. 2003) found that PA results are relatively insensitive to the uncertainty in room closure and room porosity. The conclusions of the separate PA are summarized in Section MASS-21.0 of this appendix.

MASS-7.1 Flow Interactions with the Creep Closure Model

The dynamic effect of halite creep and room consolidation on room porosity is modeled only in the waste disposal region. Other parts of the repository, such as the experimental region and the operations region, are modeled assuming fixed (invariant with time) properties. In these regions, the permeability is held at a fixed high value representative of unconsolidated material, while the porosity is maintained at relatively low values associated with highly consolidated material. This combination of low porosity and high permeability is assumed to conservatively overestimate flow through these regions and minimize the capacity of this material to store fluids, thus maximizing the release to the environment. To examine the acceptability of this assumption, a screening analysis (Vaughn, Lord, and MacKinnon 1995c) evaluated the effect of including closure of the experimental region and operations region. In this analysis, consolidation of the

experimental region and operations region was implemented in BRAGFLO by relating pressure and time to porosity using a porosity-surface method. The porosity surface for the experimental region and operations region differs from the surface used for consolidation of the disposal room and is based on an empty excavation (see Appendix PORSURF-2009). The screening analysis showed that disregarding dynamic closure of the experimental region is acceptable because it is conservative: lower releases occur when closure of the experimental region and operations region is computed compared to simulations with time-invariant high permeability and low porosity.

MASS-7.2 Flow Interactions with the Gas Generation Model

Gas generation affects repository pressure, which in turn is an important parameter in other processes such as two-phase flow, creep closure, and fracturing of the interbeds and DRZ. Gas-generation processes considered in PA calculations include anoxic corrosion and microbial degradation. Radiolysis is excluded from PA calculations on the basis of laboratory experiments and a screening analysis (Vaughn et al. 1995) that concluded that radiolysis does not significantly affect repository performance.

In modeling gas generation, the effective liquid in a computational cell is the computed liquid in that cell plus an adjustment for the uncertainty associated with wicking by the waste (see Appendix PA-2009, Section PA-4.2.6). Capillary action (wicking) is the ability of a material to carry a fluid by capillary forces above the level it would normally seek in response to gravity. Because the current gas-generation model computes substantially different gas-generation rates depending on whether the waste is wet or merely surrounded by water vapor, the physical extent of wetting could be important. A screening analysis (Vaughn, Lord, and MacKinnon 1995d) examined wicking and concluded that it should be included in PA calculations.

The baseline gas-generation model in BRAGFLO accounts for corrosion of iron and microbial degradation of cellulose and possibly plastics and rubber. The net reaction rate of these processes depends directly on brine saturation: an increase in brine saturation will increase the net reaction rate by weighting the inundated portion more heavily and the slower humid portion less heavily. To simulate the effect of wicking on the net reaction rate, an effective brine saturation, which includes a wicking saturation contribution, is used to calculate reaction rates rather than the actual brine saturation. To account for uncertainty in the wicking saturation contribution, this contribution was sampled from a uniform distribution from 0.0 to 1.0 for each BRAGFLO simulation in the analysis.

MASS-7.3 CRA-2009 Flow Interactions with the Gas-Generation Model Changes

The assumptions for brine availability were changed in BRAGFLO Version 6.0 to account for brine-consuming reactions. Brine-consuming reactions such as anoxic corrosion tend to dry out the waste-filled regions of the repository. The former BRAGFLO code and underlying models could not simulate completely dry cells in the grid. To accommodate brine-consuming reactions and allow the code to run, BRAGFLO Version 6.0 includes a lower cut off in brine saturation for waste-filled regions in the repository, representing a numerically dry condition. At this cut-off saturation, biodegradation and iron corrosion ceases. This modification is explained fully in

Section 5.2.2 of Nemer and Clayton (2008). BRAGFLO version 6.0 was used in the CRA-2009 PA; older versions of the code were used in previous PAs.

MASS-8.0 Gas Generation

The gas generation model represents the possible generation of gas in the repository by corrosion of steel and microbial degradation of CPR materials. The CRA-2009 uses the CRA-2004 PABC gas generation modeling assumptions. Although the amount of the excess MgO engineered barrier emplaced in the repository has been reduced from 1.67 to 1.2, the PA methodology does not account for any excess material in the modeling assumption and therefore no changes to these assumptions are necessary. Additional discussion of this topic may be found in Appendix PA-2009, Section PA-4.2.5 and Appendix SCR-2009 (FEPs W44 through W48, W53, and N71) and the CRA-2004, Chapter 6.0, Section 6.4.3.3.

MASS-8.1 Historical Context of Gas Generation Modeling

See the CCA, Appendix MASS, Section MASS-8.1 for historical information on the development of the CCA gas-generation conceptual model.

MASS-9.0 Chemical Conditions

The chemical conditions modeling assumptions have not changed from those in the CRA-2004 PABC. The models used for chemical conditions in the repository are discussed in Appendix MgO-2009 and Appendix SOTERM-2009.

MASS-10.0 Dissolved Actinide Source Term

The dissolved An source term modeling assumptions have not changed from those in the CRA-2004 PABC. The models used for the dissolved An source term in the repository are discussed in Appendix SOTERM-2009, Section SOTERM-4.0 and Section SOTERM-5.0.

MASS-11.0 Colloidal Actinide Source Term

The colloidal An source term modeling assumptions have not changed from those in the CRA-2004 PABC. The models used for the colloidal An source term are discussed in Appendix SOTERM-2009, Section SOTERM-3.8.

MASS-12.0 Shafts and Shaft Seals

The shafts and shaft seals modeling assumptions have not changed from those in the CRA-2004 PABC. The models used for shafts and shaft seals are discussed in the CRA-2004, Appendix PA, Attachment MASS, Section MASS-12.0.

MASS-13.0 Salado

The far-field Salado modeling assumptions used in the CRA-2009 are the same as those used in the CRA-2004 PABC. No changes have been made to these modeling assumptions for the CRA-2009 PA. The purpose of this model is to reasonably represent the effects of fluid flow in the Salado on long-term performance of the disposal system. The conceptual model is also discussed in the CRA-2004, Chapter 6.0, Section 6.4.5. The Salado fluid flow model represented in the CRA-2004 PABC is also used in the CRA-2009 PA (Nemer and Clayton 2008).

Fluid flow in the Salado is considered in the conceptual model of long-term disposal system performance for several reasons. First, some liquid could move from the Salado to the repository because of the considerable gradients that can form for liquid flow inward to the repository. This possibility is important because such fluid can affect creep closure, gas generation, An solubility, and other processes occurring in the repository. Second, gas generated in the repository is thought to be capable of fracturing the Salado interbeds under certain conditions, creating increased permeability channels that could be pathways for lateral transport. The lateral transport pathway in intact Salado is also modeled, but it is considered unlikely to result in any significant radionuclide transport to the accessible environment boundary.

The fundamental principle in the conceptual model for fluid flow in the Salado is that it is a porous medium within which gas and brine can both be present and mobile (two-phase flow), governed by conservation of energy and mass and by Darcy's Law for their fluxes (see Appendix PA-2009, Sections PA-4.2). Consistent with typical concepts of two-phase flow, each phase can affect the other by impeding flow because of partial saturation (relative permeability effects) and by affecting pressure by capillary forces (capillary pressure effects). It was originally assumed that no waste-generated gas is present before repository closure. However, during the EPA completeness review of the CRA-2004, the representation of the gas-generation rate was changed for the CRA-2004 PABC (Cotsworth 2005). The repository was precharged after closure to represent the short-term, but initially faster, microbial gas-generation rate (see Section MASS-8.0 and Leigh et al. 2005, Section 2.3). Future states are modeled as producing gas by corrosion and microbial activities. Should high pressure develop over the regulatory period, it is allowed to access MBs in the Salado.

Some variability in composition exists between different horizons of the Salado. The largest differences occur between the anhydrite-rich layers called interbeds and those dominated by halite. Within horizons dominated by halite, composition varies from nearly pure halite to halite plus several percent other minerals, in some instances including clay (see the CCA, Chapter 2.0, Section 2.1.3.4). The Salado is modeled as impure halite except for those interbeds that intersect the DRZ near the repository. This conceptual model and an alternative model that explicitly represented all stratigraphically distinct layers of the Salado near the repository (Christian-Frear and Webb 1996) produced similar results.

From other modeling and theoretical considerations, flow between the Salado and the repository is expected to occur primarily through interbeds that intersect the DRZ. Because of the large surface areas between the interbeds and surrounding halite, the interbeds serve as conduits for the flow of brine in two directions: from halite to interbeds to the repository, or, for brine flowing out of the repository, from the repository into interbeds and then into halite. Because the

repository is modeled as a relatively porous and permeable region, brine is considered most likely (but not constrained) to leave the repository through MB 139 below the repository because of the effect of gravity. If repository pressures become sufficiently high, gas is modeled to exit the repository via the MBs.

The effect of gravity may also be important in the Salado because of the slight and variable natural stratigraphic dip. For long-term performance modeling, the dip in the Salado within the domain is taken to be constant and 1 degree from north to south.

Fluid flow in the Salado is conceptualized as occurring either convergently into the repository or divergently from it, as discussed in detail in the CRA-2004, Chapter 6.0, Section 6.4.2.1. Because the repository is not conceptualized as homogeneous, implementing a geometry for the conceptual model of convergent or divergent flow in the Salado is somewhat complicated and is discussed in the CRA-2004, Chapter 6.0, Section 6.4.2.1.

The conceptual model for Salado fluid flow has primary interactions with three other conceptual models. The interbed fracture conceptual model allows porosity and permeability of the interbeds to increase as a function of pressure. The repository fluid flow model is directly coupled to the Salado fluid flow model by the governing equations of flow in BRAGFLO (in the governing equations of the mathematical model, they cannot be distinguished), and it differs only in the region modeled and the parameters assigned to materials. The Salado model for An transport is directly coupled to the conceptual model for flow in the Salado through the process of advection. Additional information on the treatment of the Salado in PA is found in Appendix PA-2009, Section PA-4.2.

MASS-13.1 High Threshold Pressure for Halite-Rich Salado Rock Units

An important parameter used to describe the effects of two-phase flow is threshold pressure, which helps to determine the ease with which gas can enter a liquid-saturated rock unit. For a brine-saturated rock, the threshold pressure is defined as "equal to the capillary pressure at which the relative permeability to the gas phase begins to rise from its zero value, corresponding to the incipient development of interconnected gas flow paths through the pore network" (Davies 1991, p. 9).

The threshold pressure, as well as other parameters used to describe two-phase characteristics, has not been measured for halite-rich rocks of the Salado. The Salado, however, is thought to be similar in pore structure to rocks for which threshold pressures have been measured (Davies 1991). Based on this observation, Davies (1991) postulated that the threshold pressure of the halite-rich rocks in the Salado could be estimated if an empirical correlation exists between rocks postulated to have similar pore structure.

Davies developed a correlation between threshold pressure and intrinsic permeability applicable to the Salado halites. A similar correlation was developed for Salado anhydrites; subsequent testing confirmed that the correlation predicted threshold pressures accurately. The correlation developed by Davies predicts threshold pressures in intact Salado halites on the order of 20 MPa or greater (Davies 1991). This threshold pressure predicted by correlation is much higher than

that expected to persist in the repository, so that for all practical and predictive purposes, no gas will flow into intact Salado halites (see the CRA-2004, Chapter 6.0, Section 6.4.5.1).

Because threshold pressure helps control the flow of gas, and because the greatest volume of rock in the Salado is rich in halite, a high threshold pressure effectively limits the volume of gas that can be accommodated in the pore spaces of the intact host formation. Thus, high threshold pressure is considered conservative, because if gas could flow into the pore spaces of intact Salado halite, repository pressures could be reduced dramatically.

MASS-13.2 Historical Context of the Salado Conceptual Model

See the CCA, Appendix MASS, Section MASS-13.2 for the historical information relating to the CCA Salado conceptual model. The Salado conceptual model is unchanged for the CRA-2009 PA.

MASS-13.3 The Fracture Model

The fracture model assumptions have not changed from those in the CRA-2004 PABC. The purpose of this model is to alter the porosity and permeability of the anhydrite interbeds and the DRZ if their pressure approaches lithostatic, simulating some of the hydraulic effects of fractures with the intent that unrealistically high pressures (in excess of lithostatic) do not occur in the repository or disposal system. The conceptual model is also discussed in the CRA-2004, Chapter 6.0, Section 6.4.5.2. The fracture model assumptions have not changed from those in the CRA-2004 PABC.

In the 1992 preliminary PA, repository pressures were shown to greatly exceed lithostatic pressure if a large quantity of gas was generated. Pressures within the waste repository and surrounding regions were predicted to be roughly 20 to 25 MPa. It was expected that fracturing within the anhydrite MBs would occur at pressures slightly above lithostatic pressure. An expert panel on fractures was convened to develop the conceptual bases for the fracturing within the anhydrite MBs.

Two parametric behaviors must be quantified in the conceptual model. First, the change of porosity with pressure in the anhydrite MBs must be specified. This is done with a relatively simple equation, described in Appendix PA-2009, Section PA-4.2.4, that relates porosity change to pressure change using an assumption that the fracturing can be thought of as increasing the compressibility of interbeds. Parameters in the model are treated as fitting parameters and have little relation to physical behavior except that they affect the porosity change. The second parametric behavior is the change of permeability with pressure, which is incorporated by a functional dependence on the porosity change. It is assumed that a power function is appropriate for relating the magnitude of permeability increase to the magnitude of porosity increase. The parameter in this power function, an exponent, is also treated as a fitting parameter and can be set so that the behavior of permeability increase with porosity increase fits the desired behavior.

The fracture enhancement model assumes fracture propagation is uniform in the lateral direction to flow within the MBs in the absence of dip. The 1-degree dip modeled in BRAGFLO may affect fracture propagation direction; however, within the accuracy of the finite difference grid, a

fracture will develop radially outward. This would not account for fracture fingering or a preferential fracturing direction; however, no existing evidence supports heterogeneous anhydrite properties that would contribute to preferential fracture propagation. This evidence is discussed in the CCA, Appendix MASS, Attachment 13-2.

The maximum enhanced fracture porosity controls the storativity within the fracture. The extent of the migration of the gas front into the MB is sensitive to this storativity. The additional storativity caused by porosity enhancement will mitigate gas migration within the MB. The enhancement of permeability by MB fracturing will make the gas more mobile and will contribute to longer gas-migration distances. Thus the effects of porosity enhancement at least partially counteract the effects of permeability enhancement in affecting the gas-migration distances.

Because intact anhydrite is partially fractured, the pressure at which porosity or permeability changes are initiated is close to the initial pressure within the anhydrite. The fracture treatment within the MBs will not contribute to early brine drainage from the MB because the pressures at these times are below the fracture initiation pressure.

The input data to the interbed fracture model (see Fox 2008, Table 30, Table 31, and Table 32) were chosen deterministically to produce the appropriate pressure and porosity response as predicted by a linear elastic fracture mechanics model, as discussed in Mendenhall and Gerstle (1993).

MASS-13.4 Flow in the DRZ

Modeling assumptions relating to flow in the DRZ have not changed from those in the CRA-2004 PABC. The conceptual model for the DRZ around the waste disposal, operations, and experimental regions has been chosen to provide a reasonably conservative estimate of fluid flow between the repository and the intact halite and anhydrite MBs. The conceptual model is also discussed in the CRA-2004, Chapter 6.0, Section 6.4.5.3.

The conceptual model implemented in the CCA PA used values for the permeability and porosity of the DRZ that did not vary with time. A screening analysis examined an alternative conceptual model for the DRZ in which permeability and porosity changed dynamically in response to changes in pressure (Vaughn, Lord, and MacKinnon 1995e). This analysis implemented a fracturing model in BRAGFLO for the DRZ. This fracturing model is used in the existing anhydrite interbed model. In this model, formation permeability and porosity depend on brine pressure, as described by Freeze, Larsen, and Davies (1995, pp. 2-16 through 2-19) and Appendix PA-2009, Section PA-4.2.4. This model permits the representation of two important formation-alteration effects. First, pressure buildup caused by gas generation and creep closure within the waste will slightly increase porosity within the DRZ and offer additional fluid storage with lower pressures. Second, the accompanying increase in formation permeability will enhance fluid flow away from the DRZ. Because an increase in porosity tends to reduce outflow into the far field, parameter values for this analysis were selected so that the DRZ alteration model greatly increases permeability while only modestly increasing porosity.

Two basic scenarios were considered in the screening analysis by Vaughn, Lord, and MacKinnon (1995e): undisturbed repository performance and disturbed repository performance. Both scenarios included a 1-degree formation dip downward to the south. Intrusion event E1 is considered in the disturbed scenario and consists of a borehole that penetrates the repository and pressurized brine in the underlying Castile. Two variations of intrusion event E1 were examined: E1 updip and E1 downdip. In the E1 updip event, the intruded panel region was located on the north end of the waste disposal region, whereas in the E1 downdip event, the intruded panel region was located on the south end of the disposal region. These two different geometries permitted evaluation of the possibility of increased brine flow into the panel region and the potential for subsequent impacts on contaminant migration. To incorporate the effects of uncertainty in each case (E1 updip, E1 downdip, and undisturbed), a Latin hypercube sample (LHS) size of 20 was used, for a total of 60 simulations. To assess the sensitivity of system performance on formation alteration of the DRZ, conditional CCDFs of normalized contaminated brine releases were constructed and compared with the corresponding baseline model conditional CCDFs that were computed with constant DRZ permeability and porosity values. Based on comparisons between conditional CCDFs, computed releases to the accessible environment were determined to be essentially equivalent between the two treatments. Since the two configurations were determined to have essentially equivalent impacts on releases, the intrusion borehole was assumed to intrude in the down-dip or south side of the repository where it is assumed brine would more readily accumulate (see Figure MASS-3).

Preliminary PAs considered alternative conceptual models that allowed for some lateral extent of the DRZ into the halite surrounding the waste disposal region and for the development of a transition zone between anhydrites A and B and MB 138 (WIPP Performance Assessment 1993, Volume 4, Figure 4.1-2 and Figure 5.1-2; and Davies, Webb, and Gorham 1992; and Gorham et al. 1992). The transition zone was envisioned as a region that had experienced some hydraulic depressurization and perhaps some elastic stress relief because of the excavation, but probably no irreversible rock damage and no large permeability changes. Modeling results indicated that including the lateral extent of the DRZ had no significant effect on fluid flow. Communication vertically to MB 138 was thought to be a potentially important process, however, and the model adopted for PA assumes that the DRZ extends upward to MB 138 and permeability is sampled over the same range used in the CCA PAVT. This representation continues to be used in the CRA-2009 PA.

MASS-13.5 Actinide Transport in the Salado

The An transport modeling assumptions have not changed from those in the CRA-2004 PABC. The purpose of this model, implemented in the code NUTS, is to represent the transport of actinides in the Salado. This model is also discussed in the CRA-2004, Chapter 6.0, Section 6.4.5.4 and Appendix PA-2009, Section PA-4.3.4.

Actinide transport in the Salado is conceptualized as occurring only by advection, or movement of material through the bulk flow of a fluid, through the porous medium described in the Salado hydrology conceptual model. Advection is a direct function of fluid flow, which is discussed in the conceptual model for Salado fluid flow. Other processes that might disperse actinides, such as diffusion, hydrodynamic dispersion, and channeling in discrete fractures, are not included in

the conceptual model. Since these processes will reduce An transport, it is conservative to ignore these processes.

To model radionuclide transport in the Salado, NUTS takes as input BRAGFLO's velocity field, pressures, porosities, saturations, and other model parameters (including geometrical grid, residual saturation, material map, brine compressibility, and time step) averaged over a given number of time steps (20 for the CRA-2009 PA calculations). NUTS then models the transport of radionuclides within all the regions for which BRAGFLO computes brine and gas flow. The brine must pass through some part of the repository at some point during the 10,000-year regulatory period if it is to become contaminated. Radioactive constituents of the waste in the repository are assumed to dissolve into the brine while the brine is in the repository; the radionuclides are then transported by advection to other regions outside the repository. Consequently, the results of NUTS are subject to all the uncertainties associated with BRAGFLO's conceptual model and parameterization, and are presented in Appendix PA-2009. Details of the source term, which specifies the types and amounts of radionuclides that are assumed to come into contact with the waste, are discussed in Appendix SOTERM-2009, Section SOTERM-3.1 and Table SOTERM-6.

NUTS neglects molecular dispersion. For materials of interest in the WIPP repository system, molecular diffusion coefficients are, at most, on the order of 4×10^{-10} m^2 per second. Thus, the simplest scaling argument using a time scale of 10,000 years leads to a molecular diffusion (that is, mixing) length scale of approximately 33 ft (10 m), which is negligible compared to the lateral advection length scale of roughly 7,874 ft (2,400 m) (the lateral distance from the repository to the accessible environment).

NUTS also neglects mechanical dispersion (see the CRA-2004, Chapter 6.0, Section 6.4.5.4.2). Dispersion is quantified by dispersivities, which are empirical tensor factors proportional to flow velocity (to within geometrical factors related to flow direction). They account for both the downstream and cross-stream spreading of local extreme values in concentration of dissolved constituents. Physically, the spreading is caused by the fact that both the particle paths and velocity histories of once-neighboring particles can be vastly different because of material heterogeneities characterized by permeability variations. These variations arise from the irregular cross-sectional areas and tortuous inhomogeneous, anisotropic connectivity between pores. Because of its velocity dependence, the transverse component of mechanical dispersivity tends to transport dissolved constituents from regions of relatively rapid flow (where mechanical dispersion has a larger effect) to regions of slower flow (where mechanical dispersion has a smaller effect). In the downstream direction, dispersivity merely spreads constituents in the flow direction. Conceptually, ignoring lateral spreading assures that dissolved constituents will remain in the rapid part of the flow field, which assures their transport toward the boundary. Similarly, ignoring longitudinal dispersivity ignores the elongation of a feature in the flow direction, which would delay the arrival of radionuclide constituents at the accessible environment. However, because the EPA release limits are time-integrated measures, the exact time of arrival is unimportant for constituents that arrive at the accessible environment, so long as arrival occurs within the assessment period (10,000 years).

NUTS conservatively disregards sorptive and other retarding effects throughout the entire flow region even though retardation must occur at some level within the repository, the MBs, and the

anhydrite interbeds, and especially in zones with clay layers or clay as accessory minerals. Advection is, therefore, the only transport mechanism considered in NUTS. Because the Darcy flows are given by BRAGFLO to NUTS as input, the maximum solubility limits for combined dissolved and colloidal components are the most important NUTS parameters. These components are described in Appendix SOTERM-2009, Section SOTERM-5.0.

MASS-14.0 Geologic Units above the Salado

The modeling assumptions of the geologic units above the Salado have not changed from those in the CRA-2004 PABC. The model for geologic units above the Salado was developed to provide a reasonable and realistic basis for simulations of fluid flow within the disposal system and detailed simulations of groundwater flow and radionuclide transport in the Culebra. The conceptual model for these units is also discussed in the CRA-2004, Chapter 6.0, Section 6.4.6.

The conceptual model used in PA for the geologic units above the Salado is based on the overall concept of a groundwater basin, as introduced in the CRA-2004, Chapter 2.0, Section 2.2.1.1 and in the CCA, Appendix MASS, Section MASS-14.2. The computer code SECOFL3D was originally used to evaluate the effect on regional-scale fluid flow by recharge and rock properties in the groundwater basin above the Salado (see the CCA, Appendix MASS, Attachment 17-2). However, simpler models for this region are implemented in codes used in PA. For example, in the BRAGFLO model, layer thicknesses, important material properties including porosity and permeability, and hydrologic properties such as pressure and initial fluid saturation are specified, but the model geometry and boundary conditions are not suited to groundwater basin modeling (nor is the BRAGFLO model used to make inferences about groundwater flow in the units above the Salado). In PA, the Culebra is the only subsurface pathway modeled for radionuclide transport above the Salado, although the groundwater basin conceptual model includes other flow interactions. The Culebra model implemented in PA includes spatial variability in hydraulic conductivity and uncertainty and variability in physical and chemical transport processes. Thus, the geometries and properties of units in the different models applied to the units above the Salado by the DOE are chosen to be consistent with the purpose of the model.

The MODFLOW-2000 and SECOTP2D codes are used directly in PA to model fluid flow and transport in the Culebra. The assumptions made in these codes are discussed in the CRA-2004, Chapter 6.0, Section 6.4.6.2 and the CRA-2004, Appendix PA, Attachment MASS, Section MASS-15.0.

With respect to the units above the Salado, the BRAGFLO model is used only for determination of fluid fluxes between the shaft or intrusion borehole and hydrostratigraphic units. For this purpose, it does not need to resolve regional or local flow characteristics.

The basic stratigraphy and hydrology of the units above the Salado are described in the CRA-2004, Chapter 2.0, Section 2.1.3.5, Section 2.1.3.6, Section 2.1.3.7, Section 2.1.3.8, Section 2.1.3.9, and Section 2.1.3.10 and Section 2.2.1.4. Additional supporting information is contained in the CCA, Appendices GCR, HYDRO, and SUM. Details of the conceptual model for each unit are described in the CRA-2004, Chapter 6.0, Section 6.4.6.1, Section 6.4.6.2, Section 6.4.6.3, Section 6.4.6.4, Section 6.4.6.5, Section 6.4.6.6, and Section 6.4.6.7 and additional information on units above the Salado is found in Appendix HYDRO-2009.

The representation of units above the Salado used in the CRA-2009 PA has not changed from that used in the CRA-2004 PA.

MASS-14.1 Historical Context of the Units above the Salado Model

See the CCA, Appendix MASS, Section MASS-14.1 for historical information relating to the conceptual models for units above the Salado for the CCA. The conceptual models for the units above the Salado are unchanged for CRA-2009 PA.

MASS-14.2 Groundwater-Basin Conceptual Model

The groundwater-basin conceptual model and associated modeling assumptions have not changed from those of the CRA-2004 PABC. For a discussion on the groundwater-basin conceptual model, see the CCA, Appendix MASS, Section MASS-14.2.

MASS-15.0 Flow Through the Culebra

The Culebra flow modeling assumptions have not changed from those in the CRA-2004 PABC. The conceptual model for groundwater flow in the Culebra (1) provides a reasonable and realistic basis for simulating radionuclide transport in the Culebra and (2) allows evaluation of the extent to which uncertainty about groundwater flow in the Culebra may contribute to uncertainty in the estimate of cumulative radionuclide releases from the disposal system. See the CRA-2004, Chapter 6.0, Section 6.4.6.2 for additional references to other relevant discussions on this conceptual model.

The conceptual model used in PA for groundwater flow in the Culebra treats the Culebra as a confined two-dimensional aquifer with constant thickness and spatially varying transmissivity (see the CCA, Appendix MASS, Attachment 15-7). Flow is modeled as single-phase (liquid) Darcy flow in a porous medium.

Basic stratigraphy and hydrology of the units above the Salado are described in the CRA-2004, Chapter 2.0, Section 2.1 and Section 2.2. Additional supporting information is contained in the CCA, Appendices GCR, HYDRO, and SUM.

The conceptual model for flow in the Culebra is discussed in the CRA-2004, Chapter 6.0, Section 6.4.6.2. Details of the calibration of the T fields, based on available field data, are given in Appendix TFIELD-2009, Section TFIELD-4.0. Initial and boundary conditions used in the model are given in the CRA-2004, Chapter 6.0, Section 6.4.10.2. A discussion of the adequacy of the two-dimensional assumption for PA calculations is included in the CCA, Appendix MASS, Attachment 15-7.

The principal parameter used in PA to characterize flow in the Culebra is an index parameter (the transmissivity index) used to select a single T field for each LHS element from a set of calibrated fields (see Fox 2008, Table 1), each of which is consistent with available data.

MASS-15.1 Historical Context of the Culebra Model

See the CRA-2004, Appendix PA, Attachment MASS, Section MASS-15.1 for historical information relating to the Culebra conceptual model. The conceptual model for this unit is unchanged for CRA-2009.

MASS-15.2 Dissolved Actinide Transport and Retardation in the Culebra

The purpose of this model is to represent the effects of advective transport and physical and chemical retardation on the movement of actinides in the Culebra. This conceptual model is also discussed in the CRA-2004, Chapter 6.0, Section 6.4.6.2.1. The same model is used in the CRA-2004 PABC and the CRA-2009 PA. For a historical presentation of this model, see the CRA-2004, Appendix PA, Attachment MASS, Section MASS-15.2.

MASS-15.3 Colloidal Actinide Transport and Retardation in the Culebra

The purpose of this model is to represent the effects of colloidal An transport in the Culebra. This model is also discussed in the CRA-2004, Chapter 6.0, Section 6.4.6.2.2 and the CRA-2004, Appendix PA, Attachment MASS, Attachments 15-2, 15-8, and 15-9. No changes have been made to this model since the CRA-2004. Additional information and historical information on colloidal An transport and retardation in the Culebra can be found in the CRA-2004, Appendix PA, Attachment MASS, Section MASS-15.3.

MASS-15.4 Subsidence Caused by Potash Mining in the Culebra

The mining-related modeling assumptions have not changed from those in the CRA-2004 PABC. This model incorporates the effects of potash mining in the McNutt Potash Zone on disposal system performance (see Appendix SCR-2009, FEP H13, FEP H37, and FEP H38). Provisions in Part 194 provide a conceptual model and elements of a mathematical model for these effects. The DOE has implemented the EPA conceptual model (40 CFR § 194.32(b), U.S. Environmental Protection Agency 1996) to be consistent with EPA criteria and guidance; this model is described in the CRA-2004, Chapter 6.0, Section 6.4.6.2.3. Additional information on the implementation of the mining subsidence model is available in Appendix TFIELD-2009, Section TFIELD-9.0; the CCA, Appendix MASS, Attachments 15-4 and 15-7; and Wallace (1996).

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

Mining in the McNutt has been considered in the performance of the WIPP since the original siting activities. Siting criteria for both the site abandoned in 1975 and the current site included setbacks from active mines. (See, for example, the CCA, Appendix MASS, Section MASS-2.0.) The 1980 Final Environmental Impact Statement (FEIS) for the WIPP (U.S. Department of Energy 1980, pp. 9-145 through 9-148) considered the possibility of an indirect dose arising from the effects of solution mining for potash or halite.

Mining has been included in scenario development for the WIPP since the earliest work on this topic (see U.S. Department of Energy 1980 [pp. 9-145 through 9-148], Hunter 1989, Marietta et al. 1989, Guzowski 1990, Tierney 1991, and WIPP Performance Assessment 1991). These early scenario developments considered both solution and room-and-pillar mining. The focus was generally on effects of mining outside the disposal system. In the CCA FEPs screening, solution mining was screened out during scenario development (see Appendix SCR-2009, FEP H58 and FEP H59). The two primary effects of mining considered were (1) changes in the hydraulic conductivity of the Culebra or other units, and (2) changes in recharge as a result of surface subsidence. These mining effects were not formally incorporated into quantitative assessment of repository performance in preliminary PAs.

The inclusion of mining in PA satisfies the requirements of section 194.32(b) to consider the effects of this activity on the disposal system.

MASS-16.0 Intrusion Borehole

The intrusion borehole modeling assumptions have not been changed from those in the CRA-2004 PABC. The inclusion of intrusion boreholes in PA adds to the number of release pathways for radionuclides from the disposal system. Direct releases to the surface may occur during drilling as particulate material from cuttings, cavings, and spallings are carried to the surface. Also, dissolved actinides may be carried to the surface in brine during drilling. Once abandoned, the borehole presents a possible long-term pathway for fluid flow, such as might occur between a hypothetical Castile brine reservoir, the repository, and overlying units. This topic is also addressed in the CRA-2004, Chapter 6.0, Section 6.4.7 and Appendix SCR-2009 (FEP H1 and FEP H21).

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

The cuttings, cavings, and spallings models estimate the quantity of actinides released as solids directly to the surface during drilling through the repository. The releases are caused by three mechanisms: the drill bit boring through the waste (cuttings); the drilling fluid eroding the walls of the borehole (cavings); and high repository gas pressure causing solid material failure and entrainment into the drilling fluid in the wellbore (spallings). See the CRA-2004, Chapter 6.0, Section 6.4.7.1 and references to other appendices cited in that section for additional information. Stochastic uncertainty in parameters relevant to these release mechanisms is addressed in the CRA-2004, Chapter 6.0, Section 6.4.12. The conceptual model for cuttings, cavings, and spallings is discussed in three parts because of the different processes that produce the three types of material.

Cuttings are materials removed to the surface through drilling mud by the direct mechanical action of the drill bit. The volume of waste removed to the surface is a function of the repository height and the drill bit area. The principal parameter in the cuttings model is the diameter of the drill bit (see Appendix DATA-2009, Attachment A).

Cavings are materials introduced into the drilling mud by the erosive action of circulating drilling fluid on the waste in the walls of the borehole annulus. Erosion is driven solely by the shearing action of the drilling fluid (or mud) as it moves up the borehole annulus. Shearing may be caused by either laminar or turbulent flow. Repository-pressure effects on cavings, which are negligible, are covered by the spall process. The principal parameters in the cavings model are the properties of the drilling mud, drilling rates, the drill string angular velocity, and the shear resistance of the waste. (See Fox 2008, Table 13 and Table 18, for details on the sampled parameters used in the cavings model, the drill string angular velocity, and the effective shear resistance to erosion.)

Spallings are solids introduced into the wellbore by the fluid pressure difference between the repository and the bottom of the wellbore. If the repository pressure is sufficiently high (more than about 12 MPa) relative to the well bottom hole pressure (about 8 MPa), the stress state in the repository may cause repository solids to fail in the vicinity of the wellbore. In turn, these solids may become entrained in the gas flowing toward the well, ultimately to be carried up to the land surface and constituting a release. The principal parameters in the spallings model are the gas pressure in the repository when it is penetrated and properties of the waste such as

permeability, tensile strength, and particle diameter. Because the release associated with spalling is sensitive to gas pressure in the repository, it is strongly coupled to the BRAGFLO-calculated conditions in the repository at the time of penetration.

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

Cuttings and cavings releases are straightforward. The analytical equations governing erosion (cavings) based on laminar and turbulent flow (Appendix PA-2009, Section PA-4.5) have been implemented in the code CUTTINGS_S. Using selected input based on assumed physical properties of the waste and other drilling parameters, this code calculates the final caved diameter of the borehole that intersects the waste.

The various approaches used for spallings up to the CCA PA are documented in the CCA, Appendix MASS, Section MASS-16.1.1. Since the CCA PA, the spallings model has been extensively revised and has changed fundamentally from an end-state erosional model to a mechanically based, coupled material failure and transport model (WIPP Performance Assessment 2003a). This model is implemented in the code DRSPALL. A discussion tracing the historical steps from the CCA erosional model to the current DRSPALL model can be found in the CRA-2004, Appendix PA, Attachment MASS, Section MASS-16.1.1.

MASS-16.1.2 Waste Mechanistic Properties

Waste mechanical properties used in the CRA-2009 PA are the same as those in the CRA-2004 PA and the CRA-2004 PABC. Changes to the waste mechanistic properties for CRA-2004 were previously documented in the CRA-2004, Appendix PA, Attachment MASS, Section MASS-16.1.2. Those changes involved the development of surrogate waste materials for the WIPP spallings model. Surrogate waste recipes for 50% and 100% corrosion of the Fe-based inventory were fabricated from the projected inventory of waste materials. The development of each surrogate product assumed extensive degradation of the modeled constituent (Hansen et al. 1997). Subsurface processes contributing to massive degradation of the waste taken into consideration include ample brine availability; extensive microbial activity and corrosion of metals; and an absence of cementation, mineral precipitation, and salt encapsulation.

The WIPP PA uses the parameter BOREHOLE:TAUFAIL to represent the hydrodynamic shear strength of the waste in the numerical code CUTTINGS_S (see Appendix PA-2009, Section PA-4.5). It is officially called the "effective shear strength for erosion," but it is more commonly known as the "waste shear strength." The parameter is treated as a sampled value in WIPP PA with a log-uniform distribution and a range of 0.05 to 77 Pa. This range of values was derived by DOE from literature reviews of incipient motion of seafloor or channel bed sediments—0.05 Pa corresponds to a San Francisco Bay mud—and consideration of the mean particle size of the WIPP waste as determined by an expert elicitation (Berglund 1996, Carlsbad Area Office Technical Assistance Contractor [CTAC] 1997). The lower limit of this range of values represents what is hypothesized as an extreme case of degradation of the waste and waste containers.

MASS-16.1.3 Mechanistic Model for Spall

The CRA-2009 PA uses the same spallings model that was used in the CRA-2004 PA and the CRA-2004 PABC. No changes were made to the model or implementation of the results in PA.

In the CRA-2004 PA, a new approach to modeling the WIPP spallings process was developed to address peer review concerns during the original certification process (see the CCA, Chapter 9.0, Section 9.3.1.2 and the CRA-2004, Appendix PEER-2004, Section PEER-2004 3.0). Instead of focusing on the end state after penetration, as was done in the original CCA erosional model, the new model sought to capture the system behavior from just before penetration through to the end state. In doing so, many more phenomena were included in the model. Considered in this new conceptual model was unsteady, convergent gas flow from the repository toward the wellbore that caused mechanical stress and potential failure of solids near the face of the wellbore. Pressure in the cavity at the point of penetration was balanced by the mud column in the wellbore and the repository pressure.

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

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

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

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

DRSPALL applies the fluidized bed theory to determine the mobilization of failed material to the flow stream in the wellbore. If the escaping gas velocity exceeds the minimum fluidization velocity, failed material is fluidized and entrained for transport at the land surface. If gas velocity is too low to fluidize the bedded material, the cavity size is allowed to stabilize. The spall volumes predicted by DRSPALL are based on the following conservative assumptions for material properties and for the flow geometry within the repository:

- The particle size distribution for spallings is based on a detailed analysis (Wang 1997) of data from an expert elicitation (Carlsbad Area Office Technical Assistance Contractor [CTAC] 1997). This analysis considered several limiting cases in developing a conservative distribution for mean particle size ranging from 1 millimeter to 10 cm (Hansen, Pfeifle, and Lord 2003).

- The shape factor for fluidization of particles has a potential range from 0 to 1.0. Smaller values of the shape factor denote particles that are less spherical, and, therefore, more easily

fluidized and transported in the flow. The shape factor is conservatively set to a value of 0.1 (Lord 2003).

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

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

In summary, the conservative assumptions for waste properties, the waste flow geometry, and the driller's actions provide very conservative spalling release volumes (see also Appendix PA-2009, Section PA-4.6 for a description of the spallings model, and the CRA-2004, Appendix PEER-2004, Section PEER-2004 3.0 for the results of the spallings model peer review). As stated previously, the DRSPALL calculations from the CRA-2004 PABC were also used in the CRA-2009 PA (see Appendix PA-2009, Section PA-6.7.4 and Section PA-8.5.2.1).

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

The modeling assumptions relating to the calculations of cuttings, cavings and spallings releases have not changed since the CRA-2004. As detailed in Appendix PA-2009, Section PA-6.7.5, cuttings and cavings releases for intrusions into CH-TRU waste are computed by multiplying the volume released (calculated by the code CUTTINGS_S) by the radioactivity in three independently selected waste streams, consistent with the conceptual assumption that waste streams are randomly emplaced in waste stacks that are three drums high. The effect of this assumption on PA results was examined in a separate PA (Hansen et al. 2003) in which cuttings and cavings releases were computed by assuming that each intrusion encounters only a single waste stream. The differences in repository performance (determined by comparing the mean CCDFs for releases) were determined to be minor. For more details on the analysis, see the CRA-2004, Appendix PA, Attachment MASS, Section MASS-21.0.

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

CRA-2004, Appendix PA, Attachment MASS, Section MASS-21.0. During their completeness review of the CRA-2004, the EPA requested additional DRSPALL vectors be used in the CRA-2004 PABC. Minor changes were made to the implementation of spallings results that did not change the overall modeling assumptions. These implementation changes are outlined in Leigh et al. (2005, Section 7.8).

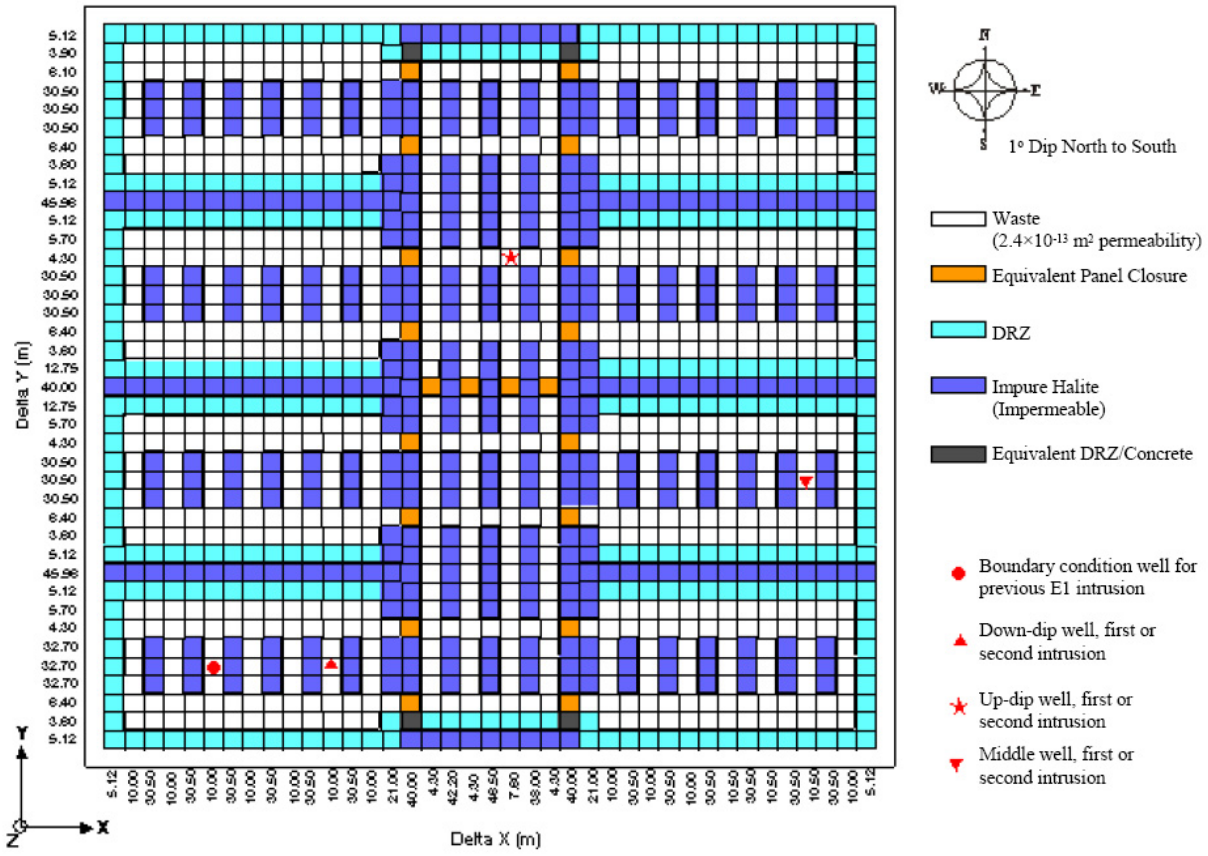
MASS-16.2 Direct Brine Releases during Drilling

The DBR modeling assumptions for the CRA-2004 PABC are used in the CRA-2009 PA. This model provides a series of calculations to estimate the quantity of brine released directly to the surface during drilling. DBRs may occur when a driller penetrates the WIPP and unknowingly brings contaminated brine to the surface during drilling (these releases are not accounted for in the cuttings, cavings, and spallings calculations, which model only the solids removed during drilling). Appendix PA-2009, Section PA-4.7 describes the DBR model used for the CRA-2009 PA. The CCA, Appendix MASS, Attachment 16-2 describes the DBR model used for the CCA PA. The conceptual model for DBRs is discussed in Appendix PA-2009, Section PA-4.7 and the CRA-2004, Chapter 6.0, Section 6.4.7.1.1.

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

To account for changes in the BRAGFLO model (see Section MASS-2.0), the implementation of the DBR model was adjusted for the CRA 2004-PA. These adjustments are also used in the CRA-2009 PA. Figure MASS-8 shows the DBR grid used in the CRA-2004 PA and the CRA-2009 PA.

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



Note: Model cells are not to scale. The actual dimensions of the grid blocks are indicated along the edge of the diagram.

Figure MASS-8. Repository-Scale Horizontal BRAGFLO Mesh Used for DBR Calculations

(2003a) provides details on the material parameters used in the DBR calculation and the rationale for the parameter values. Note that the CRA-2009 PA uses a different DBR maximum duration of 4.5 days, based on current drilling practices (see Appendix PA-2009, Section PA-4.7.8). This parameter change does not impact the modeling assumptions discussed above.

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

The long-term treatment and assumptions used to represent boreholes in the CRA-2009 PA have not changed from the treatment and assumptions used in the CRA-2004 PA. See the CRA-2004, Appendix PA, Attachment MASS, Section MASS-16.3 for the borehole modeling assumptions used in the CRA-2009 PA.

MASS-17.0 Climate Change

The purpose of this model is to allow quantitative consideration of the extent to which uncertainty about future climate may contribute to uncertainty in estimates of cumulative radionuclide releases from the disposal system. This model has not changed since the CCA and is used in the CRA-2009 PA. Consideration is limited to conditions that could result from reasonably possible natural climatic changes. The model is not intended to provide a quantitative prediction of future climate, nor is it intended to address uncertainty in system properties other than estimated cumulative radionuclide releases that may be affected by climate change. See the CRA-2004, Appendix PA, Attachment MASS, Section MASS-17.0 and Section MASS-17.1 for current and historical information on the climate change model. The implementation of this model in PA is also discussed in the CRA-2004, Chapter 6.0, Section 6.4.9 and Appendix PA, Section PA-2.1.4.6. See also the CCA, Appendix CLI for information on expected climate variability over the 10,000-year regulatory time period.

MASS-18.0 Castile Brine Reservoir

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

The representation of the Castile brine reservoir in the CRA-2009 PA has not changed from the CRA-2004 PA. However, this model is not the same as the one used in the original CCA PA. The following describes the changes to the model since the 1996 CCA PA.

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

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

The treatment of the brine reservoir for the CRA-2004 PA is different than that used in the CCA PA. The major changes to the brine reservoir representation were made by the EPA in the CCA PAVT (U.S. Environmental Protection Agency 1998b). For the CCA PAVT, the EPA defined new parameter ranges for bulk compressibility and total pore volume. The range of bulk compressibility was based on a reevaluation of field test data from the WIPP-12 borehole following the CCA (Beauheim 1997). Since the total volume of the grid cells used to represent the brine reservoir in BRAGFLO is fixed, the range of total pore volume was set by defining a range of "effective" porosity (pore volume = grid volume × effective porosity). This range of porosity values is not representative of the actual host rock. It was chosen to produce a reasonable response in the BRAGFLO model by providing a predefined range of total pore volumes based on the field tests at WIPP-12.

For the CRA-2004 PA, the DOE implemented this approach by assuming that the productivity ratio (PR) remains constant (2.0051×10^{-3} m^3/Pa). The PR is defined as:

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

where V is the grid volume of the brine reservoir (18,462,514 m^3), C_r is the bulk compressibility (2×10^{-11} to 1×10^{-10} Pa^{-1}), and ϕ is the effective porosity (0.1842 to 0.9208). To maintain a constant pore volume in the brine reservoir, the porosity range used in the CRA-2004 PA is

slightly modified from that used in the CCA PAVT because the fixed-grid volume increased slightly in the CRA-2004 BRAGFLO grid from the volume assumed in the CCA BRAGFLO grid. In this approach, bulk compressibility and effective porosity are directly proportional (Stein 2003b). See Appendix PA-2009, Section PA-4.2.10 for the details on the implementation in PA.

Basic geologic information about the Castile is given in the CRA-2004, Chapter 2.0, Section 2.1.3.3. The hydrology of the known brine reservoirs is discussed in the CRA-2004, Chapter 2.0, Section 2.2.1.2.2. The treatment of the hypothetical brine reservoir in PA is discussed in the CRA-2004, Chapter 6.0, Section 6.4.8.

MASS-18.1 Historical Context of the Castile Brine Reservoir Model

See the CCA, Appendix MASS, Attachment 18.1 for historical information on the Castile brine reservoir model.

MASS-19.0 Option D Panel Closure

The option D panel closure assumptions have not changed from those used in the CRA-2004 PABC. The certification decision by the EPA (U.S. Environmental Protection Agency 1998a) included several conditions that the DOE was required to meet. In the first of these conditions, the EPA required the DOE to implement a specific design for the panel closure system referred to as Option D and required the concrete monolith to be constructed using SMC. The DOE had included four Options (A-D) for the panel closure design using standard concrete or SMC in the CCA. The Option D design consisted of two components: a large monolith constructed of SMC and keyed into the surrounding DRZ, and an explosion wall constructed of concrete blocks, which is not keyed into the DRZ.

The PA calculations that supported the CCA and the subsequent CCA PAVT calculations included generic panel closures in the BRAGFLO grid. These generic closures were not representative of the Option D design. The generic panel closures included in the CCA PA and the CCA PAVT calculations were relatively permeable and allowed gas to flow freely between panels. In the CCA PA and the CCA PAVT calculations, a drilling intrusion into a single panel generally caused pressures in the entire repository to decrease.

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

In the CCA PA/CCA PAVT BRAGFLO grid, only two panel closures were represented. For the CRA-2004 PA and the CRA-2009, however, the DOE included an additional set of panel closures. Preliminary tests of the Option D panel closure representation (Hansen et al. 2002) concluded that Option D panel closures were effective at impeding fluid flow between panels on the order of thousands of years, but that, given enough time, pressures slowly equilibrated. These results suggest that the effect of a single intrusion event on pressures in other panels depends on the number of panel closures that lie between the intruded panel and the other panels. Therefore, the DOE decided to divide the RoR region into two regions separated by a panel closure. This panel closure represents a set of four panel closures to be located between the northern and southern internal extended panels. The south RoR represents panels directly adjacent to an intruded panel and the north RoR represents panels that are farther away from the intruded panel (two sets of panel closures lie in between).

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

closures in series and a width equal to the width of the monolith (10 m) multiplied by the number of panel closures in parallel. For instance, in Figure MASS-3, the southern panel closure in the BRAGFLO grid represents a single set of two panel closures (in parallel) that separate a single external panel from one of the two internal extended panels (9 and 10). The middle panel closure in the BRAGFLO grid represents a single set of four panel closures (in parallel) that separate the internal extended panels (9 and 10) from one another. The northern panel closure in the BRAGFLO grid represents two sets (in series) of four panel closures (in parallel) that lie between the northern edge of the waste region and the shafts.

It is assumed in the modeling that the DRZ above the concrete monolith will heal and quickly attain a state of relatively low permeability. However, it is also assumed that if pressures exceed the fracture initiation pressure (~0.2 MPa above lithostatic), the DRZ and anhydrite MB materials that intersect the waste room can fracture and allow gas or brine to circumvent the panel closures by flowing around the concrete monolith. This possibility is included in the implementation of the panel closures in the BRAGFLO by replacing the concrete monolith material with MB material everywhere the monolith intersects and cuts through the MBs. This implementation is appropriate even at low pressures because the permeability range of the concrete and the MBs is nearly equivalent. In addition, fracturing is considered in these grid elements at high pressures, allowing fluids to flow and simulating the consequence of fractures extending around the monolith.

The representation of panel closures used in the CRA-2004 PABC has not changed and this representation continues to be used in the CRA-2009 PA (see Figure MASS-6 and Appendix PA-2009, Section PA-4.2.8). Additional information on panel closure effects on repository performances can be seen in the CRA-2004 BRAGFLO Analysis Package (Stein and Zelinski 2003a and 2003b).

MASS-20.0 Summary of Clay Seam G Modeling Assumptions

One of the changes to the repository design since the CCA is the raising of the repository horizon in the southern half of the waste panels. Specifically, Panels 3, 4, 5, 6, and 9 will be excavated at an elevation approximately 2.4 m above the level of Panels 1, 2, 7, 8, and 10 and the operations and experimental areas. This change in horizon will bring the roof of the raised rooms to the level of the Clay Seam G. The change is expected to improve roof conditions and enhance operations and mine safety. The DOE submitted a planned change request to the EPA describing the change and arguing that it would have minimal impact on long-term repository performance (Triay 2000). The EPA responded to the change request in a letter (Marcinowski 2000) in which they agreed with the DOE that the effects on long-term performance would be minimal. The modeling assumptions used to represent this change are described in the CRA-2004, Appendix PA, Attachment MASS, Section MASS-20.0. No changes were made to these assumptions since the CRA-2004 PA. These assumptions have also been used in the CRA-2009 PA.

MASS-21.0 Evaluation of Waste Structural Impacts, Emplacement and Homogeneity

Waste-related modeling assumptions have not changed from those used in the CRA-2004 PABC. During the development of the CCA PA, the DOE choose to assume random placement of TRU waste in the WIPP, and developed conceptual and numerical models accordingly. The EPA reviewed these models and their results and determined that the DOE had adequately modeled random placement of waste in the disposal system. Since the CCA, additional information about the waste and its emplacement has emerged, requiring the assumption of random placement to be reevaluated. The waste inventory estimates were updated since the CCA PA (see the CRA-2004, Appendix TRU WASTE and Leigh, Trone, and Fox 2005 for the CRA-2004 PABC waste updates), resulting in different estimates of important waste components, such as CPR materials. Additionally, the CCA PA assumed that all waste could be modeled as if the waste was emplaced in 55-gallon (gal) drums. However, the DOE is emplacing waste using several different types of waste containers, including standard waste boxes and pipe overpacks. Waste has been shipped to WIPP in campaigns from the generator sites, resulting in waste emplacement that appears inconsistent with the representation of the waste as a homogeneous material. Finally, the DOE is emplacing waste types, such as supercompacted waste, that were not considered in the CCA inventory (U.S. Department of Energy 2002).

Many important waste characteristics, such as the radionuclide content and the mass of CPR materials, are directly incorporated in PA by means of waste material parameters. These parameters have been updated with the inventory updates (see Leigh and Trone 2005b, and Leigh, Trone, and Fox 2005) and thus were represented in the CRA-2004 PABC and the CRA-2009 PA. However, the PAs for compliance applications have not specifically accounted for heterogeneity in waste materials or in waste containers. At the INL, for instance, debris waste is volume-reduced by supercompaction, resulting in a very dense waste form containing a high concentration of CPR material. In addition, the Pu residues from the Rocky Flats Environmental Technology Site were packaged in pipe overpacks, which are more rigid than the typical 55-gal drum assumed in the CCA. Additionally, in accordance with the requirements of 40 CFR § 194.24(d) (U.S. Environmental Protection Agency 2004), all PAs have assumed that waste is emplaced in a random or homogeneous manner. Actual waste emplacement is determined by the availability of waste at generator sites and the shipping schedules. Pipe overpacks occupy about 43% of the containers emplaced in Panel 1, suggesting that actual emplacement will not be statistically random.

As a result of this new information and these changes, the DOE performed analyses (Hansen et al. 2003) to determine if the modeling assumptions used in PA continue to adequately represent the waste. The analysis reported in Hansen et al. (2003) focused on potential effects of supercompacted waste and waste in pipe overpacks on repository performance. Both waste types are structurally stiffer than the generic waste model used in the CCA PA, and the supercompacted waste in particular has high concentrations of CPR materials. The analysis began with a systematic reevaluation of the baseline FEPs to identify specific components of PA that could be affected by supercompacted waste. The reassessment concluded that the FEPs "screened in" were adequate to represent the variety of waste types and containers, and that none of the "screened out" FEPs should be reconsidered for implementation. The FEPs assessment

concluded that creep closure of the repository, chemical conditions of the waste, gas generation models, and waste mechanical properties could be affected by heterogeneities in the waste materials and waste containers. In addition, the DOE determined that the assumption of random waste emplacement should be reevaluated.

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

Chemical conditions were also reexamined under a range of possible waste arrangements. The assessment found that, regardless of actual waste emplacement, the MgO would still be sufficient to maintain desired chemical conditions. Moreover, the constituents of supercompacted waste would not alter the reactions that determine chemical equilibrium and, consequently, no changes to An solubilities or to the gas-generation models were warranted to account for waste heterogeneity. This topic was addressed during the second recertification in response to comment G-12, in which the EPA requested that the DOE address potential effects of heterogeneous waste loading based on the assumption of homogeneous chemical conditions. The DOE's response indicated that the chemical conditions assumptions adequately addressed nonrandom waste loading (Piper 2004). This was again addressed during the evaluation of the MgO excess factor change from 1.67 to 1.20 (Reyes 2008). No changes were made to the chemical conditions model as a result of these investigations.

Supercompacted waste contains elevated amounts of CPR materials relative to other waste streams, and the future arrangement of this waste in the WIPP repository is uncertain. Thus, the analysis treated the spatial distribution of CPR materials as uncertain. However, sensitivity analysis demonstrated that uncertainty in the spatial distribution and quantity of CPR materials had little effect on PA results. This was also shown in an analysis performed during the 2004 recertification while responding to an EPA request for additional information (Response to Comment G-12, Dunagan, Hansen, and Zelinski 2004).

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

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

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

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

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

Homogeneity issues were also addressed in response to another EPA comment during the CRA-2004 completeness review. The EPA questioned in comment C-23-10 whether negating container-scale variability was a valid assumption for spallings calculations (Cotsworth 2004). In the CRA-2004 PA, spallings releases were calculated using the average radioactivity in all CH-TRU waste streams. An analysis in Vugrin (2004) compared spallings results using three randomly sampled waste streams against results using the average radioactivity over all CH-TRU waste streams. The analysis concluded that the calculation of spallings releases is not significantly affected by waste-scale variability.

The DOE continues to assume in PA that waste is randomly emplaced in the WIPP repository. The CRA-2009 PA continues to use the same waste-related modeling approaches as the CRA-2004 PABC.

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