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## 1 INTRODUCTION AND OBJECTIVES

The Waste Isolation Pilot Plant (WIPP) is a deep geologic repository developed by the U.S. Department of Energy (DOE) for the disposal of transuranic (TRU) radioactive waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth in Title 40 of the Code of Federal Regulations (CFR), Part 191. The DOE demonstrates compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194 by means of performance assessment (PA) calculations performed by Sandia National Laboratories (SNL). WIPP PA calculations estimate the probability and consequence of radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure.

PA calculations were included in DOE's 1996 WIPP Compliance Certification Application (CCA, DOE 1996), and in a subsequent Performance Assessment Verification Test (PAVT, MacKinnon and Freeze 1997a, 1997b, 1997c). Based in part on the CCA and PAVT PA calculations, the EPA certified that the WIPP met the containment criteria in the regulations and was approved for disposal of transuranic waste in May 1998 (EPA 1998). PA calculations were also an integral part of DOE's 2004 WIPP Compliance Recertification Application (CRA-2004) (DOE 2004). During their review of the CRA-2004, the EPA requested an additional PA calculation be conducted with modified assumptions and parameter values (Cotsworth 2005). This PA is referred to as the WIPP 2004 Compliance Recertification Application Performance Assessment Baseline Calculation (CRA-2004 PABC, Leigh et al. 2005a). With the EPA's recertification decision in 2006, the CRA-2004 PABC was established as the PA baseline. Continued review of the CRA-2004 PABC has shown that a number of technical changes and corrections are necessary. Furthermore, updates to parameters and improvements to the PA computer codes have been developed since the recertification.

The Land Withdrawal Act (U.S. Congress 1992) requires that the DOE apply for recertification every five years from the first receipt of waste. Thus, the DOE is required to submit no later than March 2009. The results of the analysis described herein will be included in the 2009 Compliance Recertification Application (CRA-2009) to demonstrate compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194.

This analysis plan directs the work to be performed by SNL in a PA for the WIPP repository that captures the changes introduced since the CRA-2004 PABC. This calculation will be referred to as the CRA-2009 PA. The changes from the CRA-2004 PABC that will be implemented in the CRA-2009 PA can be grouped into three areas which include:

1. Modification and improvements to:
  - a. the parameter representing the maximum flow duration for DBRs
  - b. the sampling method applied to the humid and inundated CPR degradation rates
  - c. include additional chemistry parameters
  - d. capillary pressure and relative permeability models
  - e. computer codes used in the PA.
2. Update of the drilling rate (GLOBAL:LAMBDA) as required by Title 40 CFR 194.15.

3. Error corrections:
  - a. to account for cellulose, plastic and rubber (CPR) contents in emplacement materials in the inventory
  - b. to halite/disturbed rock zone porosity parameters
  - c. to the fraction of repository volume occupied by waste
  - d. to the input files for the direct brine release (DBR) calculations and the NUTS code.

It is expected that all of the changes do not significantly impact releases and are minor, but need to be incorporated for completeness and correctness. The results of the CRA-2009 PA will be used to show the impacts

The Analysis Plan for the 2009 Compliance Recertification Application Performance Assessment, AP-132 (Vugrin and Nemer 2007) included adding the results from the Analysis Plan for the Modification of the Waste Shear Strength Parameter and Direct Brine Release Parameters, AP-131 (Kirkes and Herrick 2006) and the Analysis Plan for Prediction of the Extent and Permeability of the Disturbed Rock Zone around a WIPP Disposal Room, AP-133 (Park and Ismail 2007). This analysis plan is the product of the decision to remove of the modification to the waste shear strength parameter and the results from AP-133 to the CRA-2009 PA (Kessel 2007).

## **2 APPROACH**

The CRA-2009 PA analysis will be used to demonstrate compliance with the containment requirements according to the Certification Criteria in Title 40 CFR paragraph 194. A full set of PA calculations that include the PA updates and corrections will be executed and the results of these calculations will be compared with the CRA-2004 PABC results. The results of the CRA-2004 PABC (Leigh et al. 2005a) represent performance of the repository under the current EPA-approved PA baseline. In order to isolate the impact of the inclusion of the PA updates and corrections, the CRA-2009 PA is designed to deviate as little as possible from the CRA-2004 PABC implementation. The CRA-2009 PA will examine all aspects of repository performance that were considered in the CRA-2004 PABC analysis.

The approach used for the CRA-2009 PA will be very similar to that used for CRA-2004 PABC (Kanney and Leigh 2005). PA begins with an analysis of the Features, Events, and Processes (FEPs) that may or may not have bearing on the performance of the repository. The FEPs are screened to determine which FEPs will be accounted for in PA. These “retained” FEPs are formulated into scenarios that will be modeled. Scenarios are modeled using conceptual models that represent the physical and chemical processes of the repository. The conceptual models are implemented through a series of computer simulations and associated parameters that describe the natural and engineered components of the disposal system (e.g., site characteristics, waste forms, waste quantities, and engineered features). The computer simulations are developed from conceptual models. The results of the simulations quantify the magnitude and probability of potential releases of radioactive materials from the disposal system to the accessible environment over the 10,000-year regulatory period.

The following sections detail how the CRA-2009 PA will be implemented and particular attention is given to how the CRA-2009 PA implementation will differ from the CRA-2004 PABC.

## 2.1 Changes Relative to CRA-2004 PABC

The CRA-2009 PA will contain several updates and corrections from CRA-2004 PABC. The following sections describe how these issues will be accounted for in the CRA-2009 PA and how they differ from the CRA-2004 PABC.

### 2.1.1 Duration of Direct Brine Releases

In the WIPP PA intrusion scenarios, it is hypothesized that brine containing radionuclides could be expelled from repository to the land surface during or directly following the drilling intrusion if repository pressures and brine saturations are sufficiently high (Stoelzel and O' Brien 1996). The expelled brine volumes are termed DBRs. The duration of a DBR event is constrained by the parameters BLOWOUT:MINFLOW and BLOWOUT:MAXFLOW. The parameter BLOWOUT:MINFLOW represents the minimum DBR duration time, and the parameter BLOWOUT:MAXFLOW represents the maximum DBR duration time. For the CRA-2004 PABC the minimum and maximum DBR durations were set to 3 days and 11 days, respectively.

AP-131 (Kirkes and Herrick 2006) describes an analysis that was conducted to reexamine the values of the parameters BLOWOUT:MINFLOW and BLOWOUT:MAXFLOW. The results of the AP-131 analysis showed that the value for BLOWOUT:MAXFLOW should be decreased from 11 days to 4.5 days, while the value for BLOWOUT:MINFLOW should remain the same (Kirkes 2007). The modified DBR maximum duration parameter will be used for the CRA-2009 PA. A comparison of the DBR duration values for the CRA-2009 PA and the CRA-2004 PABC are shown in Table 1. The DBR maximum duration parameter is used by the code BRAGFLO\_DBR<sup>1</sup>.

**Table 1. DBR Duration Parameters.**

Name	Description	Analysis	Value (seconds)
BLOWOUT:MINFLOW	Minimum DBR duration	CRA-2004 PABC	2.592E+5
		CRA-2009	2.592E+5
BLOWOUT:MAXFLOW	Maximum DBR duration	CRA-2004 PABC	9.504E+5
		CRA-2009	3.888E+5

### 2.1.2 CPR Degradation Rate

The WIPP PA brine and gas flow model includes gas generation from the microbial degradation of CPR materials. The model assumes that the gas generation occurs at a given rate, for which the possible range was determined from laboratory experiments. The inundated microbial

<sup>1</sup> The code BRAGFLO (Brine And Gas FLOW) can be run in two different modes. In the DBR mode, the code calculates a volume of brine containing dissolved radionuclides that could be released to the land surface directly following a drilling intrusion into the repository. The term "BRAGFLO\_DBR" is used to denote when the code is run in DBR mode.

degradation rate for cellulose, WAS\_AREA:GRATMICI, is represented by a uniform distribution between  $3.08269 \times 10^{-11}$  and  $5.56921 \times 10^{-10}$  moles/kg/s, while the humid microbial degradation rate for cellulose, WAS\_AREA:GRATMICH, is represented by a uniform distribution between 0 and  $1.02717 \times 10^{-9}$  moles/kg/s. Although the parameters are nominally independent, there is a physical connection between the two distributions, as the humid rate can not be faster than the inundated rate, and therefore should have a lower value than inundated rate in any given vector.

In general, no correlation was imposed between the inundated and humid microbial cellulose degradation rate, and so it is possible that the Latin Hypercube Sampling code, LHS, may sample a humid rate that is higher than the inundated rate for a single vector. For the CRA-2004 PABC, if the sampled humid rate was higher than the inundated rate for a single vector, the humid rate was set to be equal to the inundated rate in a preprocessing step for the BRAGFLO calculations. For the CRA-2009 PA, a conditional relationship will be applied such that the sampled inundated rate is used as the maximum, in the sampling for the humid rate. This conditional relationship still does not impose a correlation between the humid and inundated rates. The conditional relationship will be applied during the LHS process, as this is an improvement which will facilitate sensitivity studies. A utility will be developed that post-processes the LHS output file and update the output file to account for this conditional relationship, that will then be used by the code POSTLHS.

### *2.1.3 Additional Chemistry Parameters*

BRAGFLO version 5.0 was used for the CRA-2004 PABC. BRAGFLO version 6.0 was developed to incorporate additional capabilities and flexibility (Nemer 2007a). This code includes a few additional minor modifications, such as rate smoothing algorithms and use of effective saturations, to improve code stability. These changes are detailed in Nemer (2007c, 2007f, 2007g).

One of the added capabilities incorporated into BRAGFLO version 6.0 (that will not be used for this analysis because of the aforementioned reasons) is to be able to model the MgO hydration reaction. Furthermore, additional flexibility was added to the CPR degradation, iron corrosion, iron sulfidation and MgO carbonation reactions that were already present (BRAGFLO version 6.0 has all the same functionality as version 5.0 (Nemer 2007h)). This necessitated the introduction of additional parameters used to describe the reactions, which are shown in Table 2 through Table 8 (Clayton and Vugrin 2007). In the CRA-2004 PABC, the stoichiometric coefficients for gas, water and iron in the iron corrosion reaction and for gas, water and cellulose in the CPR degradation reaction were calculated in ALGEBRACDB, while for the CRA-2009 PA, they will be entered as the parameters shown in Table 2 and Table 3. The parameters entered into the database are the same as were calculated in ALGEBRACDB for the CRA-2004 PABC. Although the parameters in Table 4 through Table 8 have been added, for the CRA-2009 PA they are set to zero in the PREBRAG input file to deactivate the other reactions. This causes BRAGFLO version 6.0 to use the same reaction set as previously used in BRAGFLO version 5.0. Therefore, the addition of the parameters shown in Table 2 through Table 8 will not change predicted releases, as demonstrated in Nemer (2007h).

**Table 2. Fe Corrosion Reaction Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value
REFCON:STCO_11	Fe Corrosion:H2 Stoichiometric Coefficient	1
REFCON:STCO_12	Fe Corrosion:H2O Stoichiometric Coefficient	-2
REFCON:STCO_13	Fe Corrosion:Fe Stoichiometric Coefficient	-1
REFCON:STCO_14	Fe Corrosion:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_15	Fe Corrosion:FeOH2 Stoichiometric Coefficient	1
REFCON:STCO_16	Fe Corrosion:FeS Stoichiometric Coefficient	0
REFCON:STCO_17	Fe Corrosion:MgO Stoichiometric Coefficient	0
REFCON:STCO_18	Fe Corrosion:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_19	Fe Corrosion:MgCO3 Stoichiometric Coefficient	0

**Table 3. Microbial Gas Generation Reaction Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value
REFCON:STCO_21	Microbial Gas Generation:H2 Stoichiometric Coefficient	0
REFCON:STCO_22	Microbial Gas Generation:H2O Stoichiometric Coefficient	0
REFCON:STCO_23	Microbial Gas Generation:Fe Stoichiometric Coefficient	0
REFCON:STCO_24	Microbial Gas Generation:Cellulosics Stoichiometric Coefficient	-1
REFCON:STCO_25	Microbial Gas Generation:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_26	Microbial Gas Generation:FeS Stoichiometric Coefficient	0
REFCON:STCO_27	Microbial Gas Generation:MgO Stoichiometric Coefficient	0
REFCON:STCO_28	Microbial Gas Generation:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_29	Microbial Gas Generation:MgCO3 Stoichiometric Coefficient	0

**Table 4. Fe(OH)<sub>2</sub> Sulfidation Reaction Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value
REFCON:STCO_31	FeOH2 Sulfidation:H2 Stoichiometric Coefficient	-1
REFCON:STCO_32	FeOH2 Sulfidation:H2O Stoichiometric Coefficient	2
REFCON:STCO_33	FeOH2 Sulfidation:Fe Stoichiometric Coefficient	0
REFCON:STCO_34	FeOH2 Sulfidation:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_35	FeOH2 Sulfidation:FeOH2 Stoichiometric Coefficient	-1
REFCON:STCO_36	FeOH2 Sulfidation:FeS Stoichiometric Coefficient	0
REFCON:STCO_37	FeOH2 Sulfidation:MgO Stoichiometric Coefficient	0
REFCON:STCO_38	FeOH2 Sulfidation:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_39	FeOH2 Sulfidation:MgCO3 Stoichiometric Coefficient	0

**Table 5. Metallic Fe Sulfidation Reaction Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value
REFCON:STCO_41	Metallic Fe Sulfidation:H2 Stoichiometric Coefficient	0
REFCON:STCO_42	Metallic Fe Sulfidation:H2O Stoichiometric Coefficient	0
REFCON:STCO_43	Metallic Fe Sulfidation:Fe Stoichiometric Coefficient	-1
REFCON:STCO_44	Metallic Fe Sulfidation:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_45	Metallic Fe Sulfidation:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_46	Metallic Fe Sulfidation:FeS Stoichiometric Coefficient	1
REFCON:STCO_47	Metallic Fe Sulfidation:MgO Stoichiometric Coefficient	0
REFCON:STCO_48	Metallic Fe Sulfidation:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_49	Metallic Fe Sulfidation:MgCO3 Stoichiometric Coefficient	0



**Table 6. MgO Hydration Reaction Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value
REFCON:STCO_51	MgO Hydration:H2 Stoichiometric Coefficient	0
REFCON:STCO_52	MgO Hydration:H2O Stoichiometric Coefficient	-1
REFCON:STCO_53	MgO Hydration:Fe Stoichiometric Coefficient	0
REFCON:STCO_54	MgO Hydration:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_55	MgO Hydration:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_56	MgO Hydration:FeS Stoichiometric Coefficient	0
REFCON:STCO_57	MgO Hydration:MgO Stoichiometric Coefficient	-1
REFCON:STCO_58	MgO Hydration:MgOH2 Stoichiometric Coefficient	1
REFCON:STCO_59	MgO Hydration:MgCO3 Stoichiometric Coefficient	0

**Table 7. Mg(OH)<sub>2</sub> Carbonation Reaction Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value
REFCON:STCO_61	MgOH2 Carbonation:H2 Stoichiometric Coefficient	0
REFCON:STCO_62	MgOH2 Carbonation:H2O Stoichiometric Coefficient	1
REFCON:STCO_63	MgOH2 Carbonation:Fe Stoichiometric Coefficient	0
REFCON:STCO_64	MgOH2 Carbonation:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_65	MgOH2 Carbonation:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_66	MgOH2 Carbonation:FeS Stoichiometric Coefficient	0
REFCON:STCO_67	MgOH2 Carbonation:MgO Stoichiometric Coefficient	0
REFCON:STCO_68	MgOH2 Carbonation:MgOH2 Stoichiometric Coefficient	-1
REFCON:STCO_69	MgOH2 Carbonation:MgCO3 Stoichiometric Coefficient	1

**Table 8. MgO Carbonation Reaction Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value
REFCON:STCO_71	MgO Carbonation:H2 Stoichiometric Coefficient	0
REFCON:STCO_72	MgO Carbonation:H2O Stoichiometric Coefficient	0
REFCON:STCO_73	MgO Carbonation:Fe Stoichiometric Coefficient	0
REFCON:STCO_74	MgO Carbonation:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_75	MgO Carbonation:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_76	MgO Carbonation:FeS Stoichiometric Coefficient	0
REFCON:STCO_77	MgO Carbonation:MgO Stoichiometric Coefficient	-1
REFCON:STCO_78	MgO Carbonation:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_79	MgO Carbonation:MgCO3 Stoichiometric Coefficient	1

The inclusion of the MgO hydration reaction required parameters to calculate the amount of MgO present (Clayton and Vugrin 2007), and the rate of the MgO hydration reaction (Deng 2007) which are shown in Table 9. Furthermore, the additional species from the additional reactions also require supplementary molecular weights, as shown in Table 10 (Clayton and Vugrin 2007). Given that for the CRA-2009 PA, the additional reactions are deactivated, the parameters in Table 9 and Table 10 will not change predicted releases, as they are not used in the calculations. An analysis showing that the additional reactions are deactivated will be included in the BRAGFLO analysis report. The additional reactions may be used in future calculations if deemed appropriate, but is mentioned here only to comprehensively describe the changes implemented in BRAGFLO version 6.0.

**Table 9. MgO Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value
WAS_AREA:MGO_EF	MgO Excess Factor: ratio of MgO to organic carbon in CPR	1.2
WAS_AREA:BRUCITE H	MgO humid hydration rate	8.9860E-02 (mol/kg/s)
WAS_AREA:BRUCITEC	MgO inundated hydration rate in ERDA-6 brine	8.7911E-02 (mol/kg/s)
WAS_AREA:BRUCITES	MgO inundated hydration rate in GWB brine	8.4314E-02 (mol/kg/s)

**Table 10. Additional Molecular Weight Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value (kg/mol)
REFCON:MW_FEOH2	Molecular Weight of Iron Hydroxide	8.9860E-02
REFCON:MW_FES	Molecular Weight of Iron Sulfide	8.7911E-02
REFCON:MW_MGO	Molecular Weight of Magnesium Oxide	4.0304E-02
REFCON:MW_MGOH 2	Molecular Weight of Magnesium Hydroxide	5.8320E-02
REFCON:MW_MGCO3	Molecular Wight of Magnesium Carbonate	8.4314E-02

Another capability included into BRAGFLO version 6.0 is the calculation of the volume of solids generated due to the chemical reactions. To enable the solid volume generation calculation, the densities of the species in the chemical reactions were added and are shown in Table 11. For the CRA-2009 PA, the calculation of the volume of solids generated due to chemical reactions is an additional output parameter and is not used in further calculations, and so will not change releases. This added capability may be used in future calculations if deemed appropriate, but is mentioned here only to comprehensively describe the changes implemented in BRAGFLO version 6.0.

**Table 11. Density Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value (kg/m <sup>3</sup> )
REFCON:DN_FE	Density of Iron	7,870
REFCON:DN_FEOH2	Density of Iron Hydroxide	3,400
REFCON:DN_FES	Density of Iron Sulfide	4,700
REFCON:DN_CELL	Density of Cellulosics Materials for BRAGFLO	1,100
REFCON:DN_MGO	Density of Magnesium Oxide	3,600
REFCON:DN_MGOH2	Density of Magnesium Hydroxide	2,370
REFCON:DN_MGCO3	Density of Magnesium Carbonate	3,050
REFCON:DN_SALT	Density of Salts for BRAGFLO	2,180

#### 2.1.4 Capillary Pressure and Relative Permeability Model

Nemer (2007c, 2007g) recommends using a modified capillary pressure and relative permeability model (REL<sub>P</sub>\_MOD=11) for open cavities. This modified model uses zero capillary pressure and removes the capillary pressure effects from the relative permeability model for the open cavities. The previous model used in the CRA-2004 PABC (REL<sub>P</sub>\_MOD=4) had zero capillary pressure, but still included capillary pressure effects on the relative permeability model. The modified model is more appropriate because capillary pressure effects are not present in an open cavity. For the CRA-2009 PA the new capillary pressure and relative permeability model for open cavities (REL<sub>P</sub>\_MOD=1) will be used for the materials

CAVITY\_1, CAVITY\_2, CAVITY\_3, CAVITY\_4, EXP\_AREA and OPS\_AREA as shown in Table 12. The modified model represents a small from the previous model.

In BRAGFLO version 6.0, a cut off saturation is used to determine when the computational cell is effectively dry and no chemical reactions are taking place. The cut off saturation is used to increase the code robustness and reduce computational time and is discussed further in Section 2.1.5 (Nemer 2007c, 2007g). A modified capillary pressure and relative permeability model (RELP\_MOD=12) was developed such that the model would be independent of the cut off saturation value (Nemer 2007c, 2007g). Only the capillary pressure part of the capillary pressure and relative permeability model was modified as the relative permeability model is unchanged from the previous model (RELP\_MOD=4). For the CRA-2009 PA the new capillary pressure and relative permeability model for areas that use the cut off saturation (RELP\_MOD=12) will be used for the materials WAS\_AREA and REPOSIT as shown in Table 12. The modified model is used to so that the results are insensitive to the cut off saturation and the results are the same as for the previous model.

**Table 12. Relative Permeability Model Parameter Values.**

Name	Description	Analysis	Value
CAVITY_1:RELP_MOD	Model number, relative permeability model	CRA-2004 PABC	4
		CRA-2009	11
CAVITY_2:RELP_MOD	Model number, relative permeability model	CRA-2004 PABC	4
		CRA-2009	11
CAVITY_3:RELP_MOD	Model number, relative permeability model	CRA-2004 PABC	4
		CRA-2009	11
CAVITY_4:RELP_MOD	Model number, relative permeability model	CRA-2004 PABC	4
		CRA-2009	11
EXP_AREA:RELP_MOD	Model number, relative permeability model	CRA-2004 PABC	4
		CRA-2009	11
OPS_AREA:RELP_MOD	Model number, relative permeability model	CRA-2004 PABC	4
		CRA-2009	11
WAS_AREA:RELP_MOD	Model number, relative permeability model	CRA-2004 PABC	4
		CRA-2009	12
REPOSIT:RELP_MOD	Model number, relative permeability model	CRA-2004 PABC	4
		CRA-2009	12

### 2.1.5 BRAGFLO Code Improvements

BRAGFLO version 6.0 was developed to incorporate additional capabilities and improve code robustness. Many of the minor changes added to improve code robustness will be included in the CRA-2009 PA, which were not part of the CRA-2004 PABC. These changes are not expected to affect releases, but are expected to increase code robustness. The effect of the changes will be addressed in the BRAGFLO analysis report.

One addition to improve code robustness is the use of a numerical parameter called the cut off saturation (Nemer 2007c, 2007g). Brine consuming reactions such as anoxic iron corrosion and MgO hydration tend to dry out the repository. As BRAGFLO is a two phase code, numerical difficulties can be encountered when one phase completely disappears. The cut off saturation is

introduced as the lower bound in saturation that is considered numerically dry. The CRA-2009 PA will use the cut off saturation to improve code robustness.

An additional rate smoothing step based on the concentration available was added to BRAGFLO version 6.0. This was added to smooth the derivative near reaction completion to increase code robustness (Nemer 2007c, 2007g). The CRA-2009 PA will use the concentration smoothing option to improve code robustness.

The capability to control initial conditions was modified for BRAGFLO version 6.0. Additional flexibility was added to the “Reset” material, which controls the initial condition for materials (Nemer 2007c, 2007g). The “Reset” material options were expanded to increase the transparency. The change also allowed the “Reset” materials to be applied to areas that are not specifically waste areas. For the CRA-2004 PABC, since the “Reset” materials were coupled with the areas that contain waste, the initial saturation of excavated area that did not include waste (shaft, panel closure materials, etc.) were set to be fully saturated during the excavation time. For the CRA-2009 PA, the additional flexibility in the “Reset” material will be used to properly set the initial condition of all the excavated area.

Furthermore, BRAGFLO version 6.0 has the added capability to change the pressure, saturation and concentrations in a material at the time of a material change. For the CRA-2009 PA this capability will be used to reset the concentrations (not the pressure or saturation of the borehole material), when an intrusion into the repository occurs. This is done for consistency, as the iron, CPR, etc. would be removed from the borehole by the intrusion.

### 2.1.6 Drilling Rate

WIPP regulations require that current drilling practices should be assumed for future inadvertent intrusions. The DOE continues to survey drilling activity in the Delaware Basin in accordance with the criteria established in 40 CFR 194.33. Local well operators are surveyed annually to provide the WIPP project with information on drilling practices, Castile brine encounters, etc. and the results are documented in a summary report (DOE 2007). The 2007 summary report shows that drilling practices have not changed from the CRA-2004 PABC with the only difference being an increase in the drilling rate (GLOBAL:LAMBDAD) to 58.5 boreholes per km<sup>2</sup> over 10,000 years or 5.85E-3 boreholes per km<sup>2</sup> per year. The updated value for the parameter GLOBAL:LAMBDAD will be included into the CRA-2009 PA as an input in the complimentary cumulate distribution function (CCDF) construction code, CCDFGF. A comparison of the values of the parameter GLOBAL:LAMBDAD for the CRA-2009 PA and the CRA-2004 PABC are shown in Table 13.

**Table 13. Drilling Rate Parameter Values.**

Name	Description	Units	Distribution	Analysis	Value
GLOBAL: LAMBDAD	Drilling rate per unit area	km <sup>-2</sup> yr <sup>-1</sup>	Constant	CRA-2004 PABC	5.25E-3
				CRA-2009	5.85E-3

### 2.1.7 Emplacement Inventory

Leigh et al. (2005b) gives a comprehensive description of the projected inventory that was used for the CRA-2004 PABC. The CRA-2009 will use the CRA-2004 PABC inventory with one set of modifications. The CRA-2004 PABC included CPR materials in the waste and container (packaging) materials (Table 14), but the CPR contents in emplacement materials were erroneously omitted from the CRA-2004 PABC (Nemer 2007d). To correct this omission, six new parameters representing the density of CPR materials in emplacement materials were created and will be used in the CRA-2009 PA. Four additional parameters were created and will be used in the CRA-2009 PA, which represent the density of cellulose and rubber materials in container (packaging) materials. Table 15 lists the names and descriptions of those ten additional parameters. The addition of the four additional parameters is done solely for book-keeping purposes since packaging materials do not contain cellulose or rubber materials, as seen by the zero values in Table 15.

**Table 14. CRA-2004 PABC Cellulose, Plastic and Rubber Parameters.**

Name	Description	Value (kg/m <sup>3</sup> )
WAS_AREA: DCELLCHW	Average density of cellulose in CH waste materials	60.0
WAS_AREA: DCELLRHW	Average density of cellulose in RH waste materials	9.3
WAS_AREA: DPLASCHW	Average density of plastic in CH waste materials	43.0
WAS_AREA: DPLASRHW	Average density of plastic in RH waste materials	8.0
WAS_AREA: DPLSCCHW	Average density of plastic in CH waste container (packaging) materials	17.0
WAS_AREA: DPLSCRHW	Average density of plastic in RH waste container (packaging) materials	3.1
WAS_AREA: DRUBBCHW	Average density of rubber in CH waste materials	13.0
WAS_AREA: DRUBBRHW	Average density of rubber in RH waste materials	6.7

**Table 15. Cellulose, Plastic and Rubber Parameters to be Created for the CRA-2009 PA.**

Name	Description	Value (kg/m <sup>3</sup> )
WAS_AREA:DCELECHW	Average density of cellulose in CH waste emplacement materials	1.22
WAS_AREA:DCELERHW	Average density of cellulose in RH waste emplacement materials	0.0
WAS_AREA: DCELCCHW	Average density of cellulose in CH waste container materials	0.0
WAS_AREA: DCELCRHW	Average density of cellulose in RH waste container materials	0.0
WAS_AREA:DPLSECHW	Average density of plastic in CH waste emplacement materials	8.76
WAS_AREA:DPLSERHW	Average density of plastic in RH waste emplacement materials	0.0
WAS_AREA:DRUBECHW	Average density of rubber in CH waste emplacement materials	0.0
WAS_AREA:DRUBERHW	Average density of rubber in RH waste emplacement materials	0.0
WAS_AREA: DRUBCCHW	Average density of rubber in CH waste container materials	0.0
WAS_AREA: DRUBCRHW	Average density of rubber in RH waste container materials	0.0

The CRA-2009 PA will use the parameters in Table 15, in addition to the CRA-2004 PABC CPR parameters. The addition of the emplacement materials will be included in the WIPP PA brine and gas flow model that is implemented in the numerical code BRAGFLO.

### 2.1.8 Halite/Disturbed Rock Zone Porosity

An error in the determination of the intact halite porosity variable, S\_HALITE:POROSITY, was discovered and reported in Parameter Problem Report 2007-002 (Ismail 2007a). The maximum of the range was taken from data reported in weight fraction without the conversion to volume fraction. Converting the maximum value from a weight fraction to a volume fraction changed the value from 0.03 to 0.0519 (Ismail 2007b). The minimum and mode values of the distribution were not affected. Furthermore, current WIPP PA practice for determining the disturbed rock zone (DRZ) porosity is to increase the S\_HALITE:POROSITY value by 0.0029. Therefore, the maximum value of the range for the DRZ\_0:POROSITY, DRZ\_1:POROSITY and DRZ\_PCS:POROSITY increased from 0.0329 to 0.0548. The CRA-2009 PA will use the corrected porosity ranges as listed in Table 16. The change in porosity will be included in the WIPP PA brine and gas flow model that is implemented in the numerical code BRAGFLO.

**Table 16. Porosity Parameter Values.**

Name	Description	Analysis	Min	Mode	Max
S_HALITE:POROSITY	Halite porosity	CRA-2004 PABC	0.001	0.01	0.03
		CRA-2009	0.001	0.01	0.0519
DRZ_0:POROSITY	DRZ porosity -5 to 0 yrs	CRA-2004 PABC	0.0039	0.0129	0.0329
		CRA-2009	0.0039	0.0129	0.0548
DRZ_1:POROSITY	DRZ porosity 0 to 10,000 yrs	CRA-2004 PABC	0.0039	0.0129	0.0329
		CRA-2009	0.0039	0.0129	0.0548
DRZ_PCS:POROSITY	DRZ above panel closure porosity -5 to 10,000 yrs	CRA-2004 PABC	0.0039	0.0129	0.0329
		CRA-2009	0.0039	0.0129	0.0548

### 2.1.9 Fraction of Repository Volume Occupied by Waste

The CRA-2009 PA will use a different value for the parameter REFCON:FVW as that parameter was modified after the CRA-2004 PABC to correct an error in its calculation. Parameter Problem Report 2007-001 (Dunagan 2007) discusses the error and how it only had a minor impact on spillings, cuttings and cavings releases. A comparison of the REFCON:FVW values for the CRA-2009 PA and the CRA-2004 PABC are shown in Table 17.

**Table 17. Fraction of Repository Volume Occupied by Waste Parameter Values.**

Name	Description	Analysis	Value
REFCON: FVW	Fraction of repository volume occupied by waste in CCDFGF model	CRA-2004 PABC	0.386
		CRA-2009	0.385

### 2.1.10 Input File Corrections

Two inconsistencies were discovered in the input files used by the ALGEBRACDB code as part of the DBR calculations. The first inconsistency involved the input file used to set up the boundary conditions for the S3 scenario calculations. The S3 scenario consists of an intrusion through the repository and a brine pocket, 1,000 years after closure. The intrusion time in the input file was incorrectly assigned the value of 350 years instead of 1,000 years. The second inconsistency entailed the limits of integration used to calculate the DBR volume. The integration limit was determined by a logic command of “if less than zero” when it should have used “if less than or equal to zero”. The CRA-2009 PA will include the corrections to the DBR calculation input files.

Two discrepancies were noted in the input files for both the NUTS and ALGEBRACDB codes as part of the Salado transport calculations. The first discrepancy comprised the incorrect definition of grid coordinates for the “North Rest of Repository”, which referenced column 35 instead of column 36. The second discrepancy related to incorrect cell number designations (1297, 1298 and 1299 instead of 1197, 1198 and 1199) used in the radionuclide transport flux calculation. The CRA-2009 PA will include the corrections to the Salado transport calculation input files.

### 2.1.11 TAUFAIL

AP-132 (Vugrin and Nemer 2007) included the incorporation of the results from AP-131 and AP-133. The CRA-2009 PA will not include the waste shear strength parameter modification discussed in AP-131, or the DRZ modifications discussed in AP-133. The lower limit of the waste shear strength parameter, BOREHOLE:TAUFAIL, was changed as a result of AP-131. As the CRA-2009 PA will not include this change, the distribution for the parameter BOREHOLE:TAUFAIL will be the same as the distribution used in the CRA-2004 PABC as shown in Table 18, and cavings releases will be identical to CRA-2004 PABC cavings releases.

**Table 18. Waste Shear Strength Parameter BOREHOLE:TAUFAIL Distributions.**

Description	Units	Analysis	Distribution	Min	Max	Median	Deviation
Effective shear strength for erosion	Pa	CRA-2004 PABC	Loguniform	0.05	77.0	1.96	17.10
		AP-131	Uniform	1.5	77.0	39.25	21.79
		CRA-2009	Loguniform	0.05	77.0	1.96	17.10

## 2.2 PA Methodology

The CRA-2009 will consist of a full set of PA compliance calculations. That is, three replicates of PA calculations, each replicate consisting of 100 vectors, will be performed. The random seeds from the CRA-2004 PABC are preserved so that results from this analysis can be compared to those from the CRA-2004 PABC on a vector-by-vector basis.

## 2.3 FEPs Re-assessment

An assessment of the FEPs baseline must be conducted to determine if the FEPs basis remains valid in consideration of changes introduced by the CRA-2009 PA. The results of this FEPs Impact Assessment will be documented in a report.

## 2.4 2006 Inventory Comparison

An updated 2006 inventory report is scheduled to be completed by Los Alamos National Laboratories – Carlsbad Operations (LANL – CO) on January 31, 2008. As part of CRA-2009, a comparison report between the updated inventory and the CRA-2004 PABC inventory will be generated. Updated inventory parameters will be calculated and compared with the parameters developed from the CRA-2004 PABC inventory report. The comparison will include differences in the inputs used in PA that are based on inventory, such as the nitrate and sulfate amounts in the waste, the input parameters for the solubility calculations, the BOREHOLE:WUF parameter, the analysis of the radionuclides that dominate releases, as well as the input parameters for the NUTS, PANEL and EPAUNI codes. Furthermore, the impact on repository performance from these updated inventory parameters will be discussed in the 2006 inventory comparison report and a summary will be included in the CRA-2009.

Discussions with LANL – CO personnel working on the updated inventory report have indicated that the quantity of ethylenediaminetetraacetate (EDTA) in the TRU waste to be emplaced in the WIPP will increase from the quantity estimated for the CRA-2004 PABC. Brush and Xiong (2005) used a mass of 25.6 kg of Sodium EDTA (the assumed solid form of EDTA in the



inventory), a molecular weight of 314.2 g/mol for Sodium EDTA, and a brine volume of 10,011 m<sup>3</sup> to calculate a dissolved EDTA concentration of  $8.14 \times 10^{-6}$  moles/liter for the FMT calculations of actinide solubilities for the CRA-2004 PABC (Brush 2005). To assess the potential impact of this increase, a bounding approach will be applied by (1) recalculating actinide solubilities with FMT using EDTA concentrations of 10, 100, and 1000 times the concentration used for the CRA-2004 PABC (all other parameters will be identical to those used for the CRA-2004 PABC); and (2) using the WIPP PA codes ALGEBRACDB, PANEL, SUMMARIZE, and CCDFGF to generate mean CCDFs for direct brine releases and total releases for the actinide solubilities calculated at each of the EDTA concentrations listed in Item 1.

## 2.5 Parameters

Table 19 lists the parameters that were created for the CRA-2009 PA and Table 20 lists parameters that are being modified from their CRA-2004 PABC values for the CRA-2009 PA. Except for the parameters listed in these tables, the CRA-2009 PA will use the same parameters and parameter values that were used for the CRA-2004 PABC (Leigh et al. 2005a).

**Table 19. CRA-2009 PA Parameters Not Used in the CRA-2004 PABC.**

Name	Description	Value (Units)
WAS_AREA:DCELECHW	Average density of cellulose in CH waste emplacement materials	1.22 (kg/m <sup>3</sup> )
WAS_AREA:DCELERHW	Average density of cellulose in RH waste emplacement materials	0.0 (kg/m <sup>3</sup> )
WAS_AREA:DCELCCHW	Average density of cellulose in CH waste container materials	0.0 (kg/m <sup>3</sup> )
WAS_AREA:DCELCRHW	Average density of cellulose in RH waste container materials	0.0 (kg/m <sup>3</sup> )
WAS_AREA:DPLSECHW	Average density of plastic in CH waste emplacement materials	8.76 (kg/m <sup>3</sup> )
WAS_AREA:DPLSERHW	Average density of plastic in RH waste emplacement materials	0.0 (kg/m <sup>3</sup> )
WAS_AREA:DRUBECHW	Average density of rubber in CH waste emplacement materials	0.0 (kg/m <sup>3</sup> )
WAS_AREA:DRUBERHW	Average density of rubber in RH waste emplacement materials	0.0 (kg/m <sup>3</sup> )
WAS_AREA:DRUBCCHW	Average density of rubber in CH waste container materials	0.0 (kg/m <sup>3</sup> )
WAS_AREA:DRUBCRHW	Average density of rubber in RH waste container materials	0.0 (kg/m <sup>3</sup> )
WAS_AREA:MGO_EF	MgO Excess Factor: ratio of MgO to organic carbon in CPR	1.2
WAS_AREA:BRUCITEH	MgO humid hydration rate	8.9860E-02 (mol/kg/s)
WAS_AREA:BRUCITEC	MgO inundated hydration rate in ERDA-6 brine	8.7911E-02 (mol/kg/s)
WAS_AREA:BRUCITES	MgO inundated hydration rate in GWB brine	8.4314E-02 (mol/kg/s)
REFCON:STCO_11	Fe Corrosion:H2 Stoichiometric Coefficient	1
REFCON:STCO_12	Fe Corrosion:H2O Stoichiometric Coefficient	-2
REFCON:STCO_13	Fe Corrosion:Fe Stoichiometric Coefficient	-1
REFCON:STCO_14	Fe Corrosion:Cellulose Stoichiometric Coefficient	0
REFCON:STCO_15	Fe Corrosion:FeOH2 Stoichiometric Coefficient	1
REFCON:STCO_16	Fe Corrosion:FeS Stoichiometric Coefficient	0
REFCON:STCO_17	Fe Corrosion:MgO Stoichiometric Coefficient	0
REFCON:STCO_18	Fe Corrosion:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_19	Fe Corrosion:MgCO3 Stoichiometric Coefficient	0
REFCON:STCO_21	Microbial Gas Generation:H2 Stoichiometric Coefficient	0
REFCON:STCO_22	Microbial Gas Generation:H2O Stoichiometric Coefficient	0
REFCON:STCO_23	Microbial Gas Generation:Fe Stoichiometric Coefficient	0

Name	Description	Value (Units)
REFCON:STCO_24	Microbial Gas Generation:Cellulosics Stoichiometric Coefficient	-1
REFCON:STCO_25	Microbial Gas Generation:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_26	Microbial Gas Generation:FeS Stoichiometric Coefficient	0
REFCON:STCO_27	Microbial Gas Generation:MgO Stoichiometric Coefficient	0
REFCON:STCO_28	Microbial Gas Generation:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_29	Microbial Gas Generation:MgCO3 Stoichiometric Coefficient	0
REFCON:STCO_31	FeOH2 Sulfidation:H2 Stoichiometric Coefficient	-1
REFCON:STCO_32	FeOH2 Sulfidation:H2O Stoichiometric Coefficient	2
REFCON:STCO_33	FeOH2 Sulfidation:Fe Stoichiometric Coefficient	0
REFCON:STCO_34	FeOH2 Sulfidation:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_35	FeOH2 Sulfidation:FeOH2 Stoichiometric Coefficient	-1
REFCON:STCO_36	FeOH2 Sulfidation:FeS Stoichiometric Coefficient	0
REFCON:STCO_37	FeOH2 Sulfidation:MgO Stoichiometric Coefficient	0
REFCON:STCO_38	FeOH2 Sulfidation:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_39	FeOH2 Sulfidation:MgCO3 Stoichiometric Coefficient	0
REFCON:STCO_41	Metallic Fe Sulfidation:H2 Stoichiometric Coefficient	0
REFCON:STCO_42	Metallic Fe Sulfidation:H2O Stoichiometric Coefficient	0
REFCON:STCO_43	Metallic Fe Sulfidation:Fe Stoichiometric Coefficient	-1
REFCON:STCO_44	Metallic Fe Sulfidation:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_45	Metallic Fe Sulfidation:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_46	Metallic Fe Sulfidation:FeS Stoichiometric Coefficient	1
REFCON:STCO_47	Metallic Fe Sulfidation:MgO Stoichiometric Coefficient	0
REFCON:STCO_48	Metallic Fe Sulfidation:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_49	Metallic Fe Sulfidation:MgCO3 Stoichiometric Coefficient	0
REFCON:STCO_51	MgO Hydration:H2 Stoichiometric Coefficient	0
REFCON:STCO_52	MgO Hydration:H2O Stoichiometric Coefficient	-1
REFCON:STCO_53	MgO Hydration:Fe Stoichiometric Coefficient	0
REFCON:STCO_54	MgO Hydration:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_55	MgO Hydration:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_56	MgO Hydration:FeS Stoichiometric Coefficient	0
REFCON:STCO_57	MgO Hydration:MgO Stoichiometric Coefficient	-1
REFCON:STCO_58	MgO Hydration:MgOH2 Stoichiometric Coefficient	1
REFCON:STCO_59	MgO Hydration:MgCO3 Stoichiometric Coefficient	0
REFCON:STCO_61	MgOH2 Carbonation:H2 Stoichiometric Coefficient	0
REFCON:STCO_62	MgOH2 Carbonation:H2O Stoichiometric Coefficient	1
REFCON:STCO_63	MgOH2 Carbonation:Fe Stoichiometric Coefficient	0
REFCON:STCO_64	MgOH2 Carbonation:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_65	MgOH2 Carbonation:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_66	MgOH2 Carbonation:FeS Stoichiometric Coefficient	0
REFCON:STCO_67	MgOH2 Carbonation:MgO Stoichiometric Coefficient	0
REFCON:STCO_68	MgOH2 Carbonation:MgOH2 Stoichiometric Coefficient	-1
REFCON:STCO_69	MgOH2 Carbonation:MgCO3 Stoichiometric Coefficient	1
REFCON:STCO_71	MgO Carbonation:H2 Stoichiometric Coefficient	0
REFCON:STCO_72	MgO Carbonation:H2O Stoichiometric Coefficient	0
REFCON:STCO_73	MgO Carbonation:Fe Stoichiometric Coefficient	0
REFCON:STCO_74	MgO Carbonation:Cellulosics Stoichiometric Coefficient	0
REFCON:STCO_75	MgO Carbonation:FeOH2 Stoichiometric Coefficient	0
REFCON:STCO_76	MgO Carbonation:FeS Stoichiometric Coefficient	0
REFCON:STCO_77	MgO Carbonation:MgO Stoichiometric Coefficient	-1
REFCON:STCO_78	MgO Carbonation:MgOH2 Stoichiometric Coefficient	0
REFCON:STCO_79	MgO Carbonation:MgCO3 Stoichiometric Coefficient	1

Name	Description	Value (Units)
REFCON:MW_FEOH2	Molecular Weight of Iron Hydroxide	8.9860E-02 (kg/mol)
REFCON:MW_FES	Molecular Weight of Iron Sulfide	8.7911E-02 (kg/mol)
REFCON:MW_MGO	Molecular Weight of Magnesium Oxide	4.0304E-02 (kg/mol)
REFCON:MW_MGOH2	Molecular Weight of Magnesium Hydroxide	5.8320E-02 (kg/mol)
REFCON:MW_MGCO3	Molecular Wight of Magnesium Carbonate	8.4314E-02 (kg/mol)
REFCON:DN_FE	Density of Iron	7870 (kg/m <sup>3</sup> )
REFCON:DN_FEOH2	Density of Iron Hydroxide	3400 (kg/m <sup>3</sup> )
REFCON:DN_FES	Density of Iron Sulfide	4700 (kg/m <sup>3</sup> )
REFCON:DN_CELL	Density of Cellulosics Materials for BRAGFLO	1100 (kg/m <sup>3</sup> )
REFCON:DN_MGO	Density of Magnesium Oxide	3600 (kg/m <sup>3</sup> )
REFCON:DN_MGOH2	Density of Magnesium Hydroxide	2370 (kg/m <sup>3</sup> )
REFCON:DN_MGCO3	Density of Magnesium Carbonate	3050 (kg/m <sup>3</sup> )
REFCON:DN_SALT	Density of Salts for BRAGFLO	2180 (kg/m <sup>3</sup> )

**Table 20. CRA-2009 PA Parameters Modified from CRA-2004 PABC Values.**

Name	Description	Application	Value
S_HALITE: POROSITY	Effective porosity	BRAGFLO	0.0519 (Max)
DRZ_0: POROSITY	Effective porosity	BRAGFLO	0.0548 (Max)
DRZ_1: POROSITY	Effective porosity	BRAGFLO	0.0548 (Max)
DRZ_PCS: POROSITY	Effective porosity	BRAGFLO	0.0548 (Max)
GLOBAL: LAMBDAD	Drilling rate per unit area	CCDFGF	5.85E-3 (km <sup>2</sup> yr <sup>-1</sup> )
REFCON: FVW	Fraction of repository volume occupied by waste in CCDFGF model	CCDFGF	0.385
BLOWOUT: MAXFLOW	Maximum DBR duration	BRAGFLO_DBR	3.888E+5 (sec)
CAVITY_1:RELP_MOD	Model number, relative permeability model	BRAGFLO	11
CAVITY_2:RELP_MOD	Model number, relative permeability model	BRAGFLO	11
CAVITY_3:RELP_MOD	Model number, relative permeability model	BRAGFLO	11
CAVITY_4:RELP_MOD	Model number, relative permeability model	BRAGFLO	11
EXP_AREA:RELP_MOD	Model number, relative permeability model	BRAGFLO	11
OPS_AREA:RELP_MOD	Model number, relative permeability model	BRAGFLO	11
WAS_AREA:RELP_MOD	Model number, relative permeability model	BRAGFLO	12
REPOSIT:RELP_MOD	Model number, relative permeability model	BRAGFLO	12

## 2.6 Calculations

As the CRA-2009 PA will use the same inventory as was used for the CRA-2004 PABC with the addition of the emplacement materials, no additional inventory calculations will be conducted other than the aforementioned inventory comparison discussed in Section 2.4. The CRA-2004 PABC inventory will be used as no new inventory report has been released as of November 30, 2007. The calculations that will be performed as a result of the updates and corrections are listed below.

### 2.6.1 Parameter Sampling: LHS

Three replicates of 100 vectors will be created using LHS. The random seed and parameter ordering from the CRA-2004 PABC will be used for the CRA-2009 PA. Use of the CRA-2004 PABC random seeds and ordering will result in identical sampled parameter values for parameters that are common to both the CRA-2004 PABC and CRA-2009 PA. As a result, the CRA-2009 PA can be compared with the CRA-2004 PABC on a vector-by-vector basis. Fifty-six subjectively uncertain parameters were sampled for the CRA-2004 PABC (Kirchner 2005a). For the CRA-2009 PA, the same parameters will be sampled and then the conditional relationship described in Section 2.1.2 will be applied.

### 2.6.2 Salado Flow: BRAGFLO

The two-phase flow code BRAGFLO simulates the brine and gas flow in and around the WIPP repository and incorporates the effects of disposal room closure, gas generation, brine consumption, and inter-bed fracturing in response to gas pressure. The results of BRAGFLO scenarios S1-S5 are used as an input of the repository conditions for radionuclide transport, DBRs and spillings releases as described in Section 2.6.4, Section 2.6.6 and Section 2.6.7. The scenario S6 is used for radionuclide transport to the Culebra as described in Section 2.6.4, but is not use for DBR or spillings releases. The CRA-2004 PABC used BRAGFLO version 5.0 for the Salado flow calculations. BRAGFLO version 6.0 was developed to incorporate additional capabilities and flexibility (Nemer 2007a). BRAGFLO version 6.0 will be used for the CRA-2009 PA.

A complete suite of calculations will be run for the CRA-2009 PA: 3 replicates, 100 vectors per replicate, and 6 scenarios (Table 21) per vector. BRAGFLO calculations will be conducted as outlined in AP-122 (Kanney and Leigh 2005). With the exception of the parameters discussed in Section 2.5, the CRA-2009 PA BRAGFLO calculations will use the same parameters that were used in the CRA-2004 PABC BRAGFLO calculations.

**Table 21. WIPP PA BRAGFLO Scenarios.**

Scenario	# of Drilling Intrusions	Time of Intrusion (Years)	Castile Brine Pocket encountered
S1	0 (Undisturbed)	NA	NA
S2	1	350	Yes
S3	1	1,000	Yes
S4	1	350	No
S5	1	1,000	No
S6	2	1,000 and 2,000	Only at 2,000

As BRAGFLO version 6.0 includes more input parameters and capabilities, an updated version of PREBRAG (8.0) was developed (Gilkey 2007). The CRA-2004 PABC used PREBRAG version 7.0 with BRAGFLO version 5.0. As the CRA-2009 PA will use BRAGFLO version 6.0, PREBRAG version 8.0 will need to be used. Furthermore, while developing test cases for BRAGFLO version 6.0, an error was encountered in POSTBRAG version 4.00 (Nemer 2007e). A dynamic array was sized incorrectly which caused some data or data labels to be written

incorrectly. POSTBRAG version 4.00A (Nemer 2007b) was developed to remedy this problem and will be used in the CRA-2009 PA.

### *2.6.3 Actinide Mobilization: PANEL*

The PANEL code calculates the quantities of actinides mobilized by colloids and as dissolved species in WIPP brines. PANEL uses actinide solubilities from the parameter database which are derived from Fracture-Matrix Transport (FMT) results. As the CRA-2009 PA will use the same inventory as was used for the CRA-2004 PABC and no changes to the geochemistry conceptual model have been made, no FMT calculations will be performed for the CRA-2009 PA. The CRA-2009 PA will use the same actinide solubilities and uncertainties that were used in the CRA-2004 PABC. Consequently, the actinide mobilization calculations for the CRA-2009 PA will be identical to CRA-2004 PABC results since their conceptual models and parameters are not affected by any of the PA updates or corrections discussed in Sections 2.1. The CRA-2004 PABC PANEL results are documented in Garner and Leigh (2005).

### *2.6.4 Salado Transport: NUTS and PANEL*

The WIPP radioisotope mobilization and decay code NUTS will be used to simulate the transport of radionuclides through the Salado Formation for scenarios S1 through S5. Since BRAGFLO results affect NUTS calculations, NUTS calculation will be run for the CRA-2009 PA according to the procedure outlined in AP-122 (Kanney and Leigh 2005), with one exception. Following the CRA-2004 PABC, the WIPP PA Alpha Computing Cluster was upgraded, and this upgrade included migrating the operating system from OpenVMS version 7.3 to OpenVMS version 8.2. The version of NUTS that was used for the CRA-2004 PABC, version 2.05A, had a time and date incompatibility with the new operating system (Gilkey 2006), so it was modified to version 2.05C. The only difference between version 2.05A and 2.05C is the change made to correct the time and date incompatibility. NUTS version 2.05C will be used for the CRA-2009 PA. An analysis of the amount of radionuclides that reach the land withdrawal boundary in the undisturbed scenario using the NUTS results will be conducted and compared with the analysis done for the CRA-2004 PABC.

Based on the characteristics of each drilling event, the intrusions were classified as no change (not significantly changing repository behavior), and E1 type (where the brine pocket is hit) or an E2 type (where the brine pocket is not hit). Radionuclide transport to the Culebra for the E1E2 intrusion combination (BRAGFLO scenario S6) is calculated by running the PANEL code in “intrusion mode” (PANEL\_INT). PANEL\_INT calculations will be run for the CRA-2009 PA according to the procedure outlined in AP-122 (Kanney and Leigh 2005).

### *2.6.5 Culebra Flow and Transport: MODFLOW and SECOTP2D*

Culebra flow and transport calculations will be identical to CRA-2004 PABC results since their conceptual models are not affected by any of the PA updates or corrections discussed in Sections 2.1. Thus, the Culebra flow and transport results from the CRA-2004 PABC will be used for the CRA-2009 PA. These results are documented in Lowry and Kanney (2005).

## 2.6.6 *Direct Solids Releases*

### 2.6.6.1 **Spallings: DRSPALL**

Implementation of the PA updates or corrections discussed in Sections 2.1 do not affect the CRA-2004 PABC DRSPALL calculations, thus, the spallings results calculated by DRSPALL for the CRA-2004 PABC will be used for the CRA-2009 PA. The CRA-2004 PABC DRSPALL results are documented in Vugrin (2005).

### 2.6.6.2 **Cuttings and Cavings: CUTTINGS\_S**

The code CUTTINGS\_S has two major functions for WIPP PA: 1) calculation of cuttings and cavings volumes from a single borehole intrusion and 2) interpolation of DRSPALL volumes to calculate spallings volumes in the scenarios for drilling intrusions. The cuttings and cavings volumes calculated for the CRA-2009 PA will be unchanged from the CRA-2004 PABC, since none of the changes discussed in Section 2.1 affect cuttings and cavings calculations. Cuttings and cavings calculations will be implemented according to the procedure outlined in AP-122 (Kanney and Leigh 2005).

Spallings volumes from a single borehole intrusion are calculated by DRSPALL at initial repository pressures of 10, 12, 14, and 14.8 MPa (Kanney and Leigh 2005). Spallings releases for the CRA-2009 PA may differ from CRA-2004 PABC due to differences in repository pressures calculated by BRAGFLO. The CRA-2009 PA will use the same procedure to interpolate DRSPALL volumes to calculate spallings volumes in the scenarios for drilling intrusions that was used for the CRA-2004 PABC (Kanney and Leigh 2005). The initial repository pressure for a given scenario, time, location, and vector will be retrieved from the BRAGFLO results, and CUTTINGS\_S will calculate a spallings volume for each scenario, time, location, and vector combination by interpolating the CRA-2004 PABC DRSPALL results using the initial pressure from the CRA-2009 BRAGFLO results.

## 2.6.7 *Direct Brine Releases: BRAGFLO\_DBR*

For WIPP PA, BRAGFLO is run in the DBR mode (BRAGFLO\_DBR) to calculate DBR volumes. BRAGFLO\_DBR calculations for the CRA-2009 PA will be run according to the procedure outlined in AP-122 (Kanney and Leigh 2005) with the following exceptions:

- 1) As discussed in Section 2.1, the DBR calculations will use modified DBR maximum duration parameter, BLOWOUT:MAXFLOW, as determined by Kirkes (2007).
- 2) Instead of PREBRAG version 7.0, BRAGFLO version 5.0 and POSTBRAG version 4.00, the codes PREBRAG version 8.0, BRAGFLO version 6.0 and POSTBRAG version 4.00A will be used for the DBR calculations as discussed in Section 2.6.2.

The two-dimensional, semi-horizontally oriented grid, which represents the vicinity of the waste panels, will be the same as that used in CRA-2004 PABC. Conditions required for the initiation of a DBR release will remain unchanged from CRA-2004 PABC, and the DBR volumes will be calculated for the same scenarios and times (Table 22).

**Table 22. Direct Brine Release Intrusion Times.**

<b>DBR Scenario</b>	<b>Intrusion Times (years)</b>
S1	100, 350, 1000, 3000, 5000, 10000
S2 & S4	550, 750, 2000, 4000, 10000
S3 & S5	1200, 1400, 3000, 5000, 10000

### 2.6.8 CCDF Construction: CCDFGF

The CRA-2009 PA will calculate CCDFs of individual vectors for total normalized releases, cuttings and cavings releases, spillings releases, DBRs, and releases from the Culebra. Mean CCDFs for each release pathway will be calculated by replicate and across all replicates. The 95% confidence limit on the mean across all replicates will also be calculated. Calculation of CCDFs will follow the CRA-2004 PABC procedure discussed in AP-122 (Kanney and Leigh 2005).

### 2.6.9 Sensitivity Analysis: STEPWISE

The CRA-2009 PA will implement sensitivity analyses for results from the major codes in a manner consistent with those employed for the CRA-2004 PABC (Kanney and Leigh 2005, Kirchner 2005b). Specifically, global sensitivity analyses will be conducted on the results from CCDFGF using the linear regression code STEPWISE. Since the primary PA updates or corrections will be implemented in the BRAGFLO calculations, additional sensitivity analyses will be performed with the BRAGFLO results. WIPP PA codes such as PCCSRC and PATTRN, as well as Commercial Off-The-Shelf (COTS) statistical software, may be used to assess the sensitivity of BRAGFLO results to input parameters.

## 2.7 Reports and Documentation

Each set of calculations discussed in Section 2.6 and its subsections will be documented in an analysis report. These reports will include

- 1) discussion of any implementation changes (parameters, modeling assumptions, etc.) relative to the corresponding CRA-2004 PABC calculations; and
- 2) analysis of results relevant to the long term performance of the repository. The analysis will include comparisons of CRA-2009 PA results with CRA-2004 PABC results.

A summary report describing the major results of the PA will also be written.

An additional record of the run control will be created for the CRA-2009 PA. This document will contain:

1. A description of the hardware platform and operating system used to perform the calculations.
2. A listing of the codes and versions used to perform the calculations.
3. A listing of the scripts used to run each calculation.
4. A listing of the input and output files for each calculation.
5. A listing of the library and class where each file is stored.
6. File naming conventions.

### 3 TASKS

The tasks, responsible personnel, and estimated task schedule are summarized below in Table 23.

**Table 23. Task List and Estimated Schedule for the CRA-2009 PA.**

Task	Description	Guiding Document	Approximate Completion Date	Responsible Individual(s)
1	Parameters			
1a	Emplacement CPR	Nemer (2007d)	Completed	
1b	Halite/DRZ Porosity	PPR 2007-002	12/5/07	Ismail
1c	Drilling Rate Update	AP-137	12/5/07	Clayton
1d	FVW	PPR 2007-001	Completed	
1e	Maximum DBR Duration	AP-131	Completed	
1f	Waste Shear Strength	AP-137	12/5/07	Clayton
2	Parameter Entry	SP 9-5	12/7/07	Long
3	Code Run Environment Preparation			
3a	Libraries Update	AP-137	12/7/07	Long
3b	Run Control Script Update	AP-137	12/7/07	Long
4	Calculations			
4a	Parameter Sampling: LHS	AP-137	12/12/07	Long
4b	Salado Flow: BRAGFLO	AP-137	12/20/07	Long
4c	Cuttings & Cavings: CUTTINGS_S	AP-137	12/21/08	Long
4d	Direct Brine Releases: BRAGFLO_DBR	AP-137	1/8/08	Long
4e	Salado Transport: NUTS & PANEL	AP-137	1/21/08	Long
4f	CCDF Construction: CCDFGF	AP-137	1/24/08	Long
4g	Sensitivity Analysis: STEPWISE	AP-137	1/31/08	Kirchner
4h	Inventory Comparison: PANEL & CCDFGF	AP-137	2/28/08	Long
5	Analysis & Documentation			
5a	Parameter Sampling: LHS	AP-137	1/24/08	Kirchner
5b	Salado Flow: BRAGFLO	AP-137	2/12/08	Nemer & Clayton
5c	Salado Transport: NUTS & PANEL	AP-137	2/25/08	Garner & Ismail
5d	Cuttings & Cavings: CUTTINGS_S	AP-137	1/30/08	Ismail
5e	Direct Brine Releases: BRAGFLO_DBR	AP-137	3/4/08	Clayton & Nemer
5f	CCDF Construction: CCDFGF	AP-137	3/25/08	Dunagan
5g	Sensitivity Analysis: STEPWISE	AP-137	3/25/08	Kirchner
5h	Run Control Document	AP-137	2/21/08	Long
5i	FEPS Re-assessment	SP 9-4	3/31/08	Kirkes
5j	2006 Inventory Comparison	AP-137	3/13/08	Dunagan
5k	AP-131 Impact Report	AP-131	12/31/07	Kirkes
5l	Summary Report	AP-137	4/15/08	Clayton



## 4 SOFTWARE

The major WIPP PA codes to be used for this analysis are listed in Table 24. These codes will be executed on the WIPP PA Alpha Cluster, which is described in Table 25. Additionally, COTS, such as MATHEMATICA®, MATLAB®, MATHCAD®, Excel®, Access®, Grapher®, or Kaleidagraph®, running on MS Windows XP®-based PC workstations may be utilized. The use of any COTS application will be verified per NP 9-1 Appendix C as appropriate.

**Table 24. Codes to be Used for the CRA-2009 PA.**

Code	Version	Build Date	Executable
ALGEBRACDB	2.35	31-JAN-1996	ALGEBRACDB_PA96.EXE
BRAGFLO	6.0	12-FEB-2007	BRAGFLO_QB0600.EXE
CCDFGF	5.02	13-DEC-2004	CCDFGF_QB0502.EXE
CCDFSUM	2.01	26-SEP-1997	CCDFSUM_QA0201.EXE
CUTTINGS_S	6.02	9-JUN-2005	CUTTINGS_S_QA0602.EXE
GENMESH	6.08	31-JAN-1996	GM_PA96.EXE
ICSET	2.22	1-FEB-1996	ICSET_PA96.EXE
LHS	2.42	18-JAN-2005	LHS_QA0242.EXE
MATSET	9.10	29-NOV-2001	MATSET_QA0910.EXE
NUTS	2.05C	24-MAY-2006	NUTS_QA0205C.EXE
PANEL	4.03	25-APR-2005	PANEL_QA0403.EXE
PATTRN	1.00	15-MAR-1999	PTN_QA0100.EXE
PCCSRC	2.21	23-MAY-1996	PCCSRC_PA96.EXE
POSTBRAG	4.00A	28-MAR-2007	POSTBRAG_QA0400A.EXE
POSTLHS	4.07A	25-APR-2005	POSTLHS_QA0407A.EXE
PREBRAG	8.0	8-MAR-2007	PREBRAG_QA0800.EXE
PRECCDFGF	1.01	7-JUL-2005	PRECCDFGF_QA0101.EXE
PRELHS	2.30	27-NOV-2001	PRELHS_QA0230.EXE
RELATE	1.43	6-MAR-1996	RELATE_PA96.EXE
STEPWISE	2.21	2-DEC-1996	STEPWISE_PA96_2.EXE
SUMMARIZE	3.01	21-DEC-2005	SUMMARIZE_QB0301.EXE

**Table 25. WIPP PA Alpha Cluster.**

Node	Hardware Type	CPU	Operating System
CCR	HP AlphaServer ES45	Alpha EV68	Open VMS 8.2
TDN	HP AlphaServer ES45	Alpha EV68	Open VMS 8.2
BTO	HP AlphaServer ES45	Alpha EV68	Open VMS 8.2
CSN	HP AlphaServer ES45	Alpha EV68	Open VMS 8.2
GNR	HP AlphaServer ES47	Alpha EV7	Open VMS 8.2
MC5	HP AlphaServer ES47	Alpha EV7	Open VMS 8.2
TRS	HP AlphaServer ES47	Alpha EV7	Open VMS 8.2
TBB	HP AlphaServer ES47	Alpha EV7	Open VMS 8.2

## 5 SPECIAL CONSIDERATIONS

The 2006 inventory comparison report described in Section 2.4 is contingent on the receipt of the 2006 inventory report from LANL – CO on January 31, 2008.

## 6 APPLICABLE PROCEDURES

All applicable WIPP QA procedures will be followed when conducting these analyses.

- Training of personnel will be conducted in accordance with the requirements of NP 2-1, *Qualification and Training*.
- Analyses will be conducted and documented in accordance with the requirements of NP 9-1, *Analyses*.
- All software used will meet the requirements laid out in NP 19-1, *Software Requirements* and NP 9-1, as applicable.
- The analyses will be reviewed following NP 6-1, *Document Review Process*.
- All required records will be submitted to the WIPP Records Center in accordance with NP 17-1, *Records*.
- New and revised parameters will be created as discussed in NP 9-2, *Parameters*.

## 7 REFERENCES

Brush, L.H. 2005. Results of Calculations of Actinide Solubilities for the WIPP Performance Assessment Baseline Calculations. Sandia National Laboratories, Carlsbad, NM. ERMS 539800.

Brush, L.H., and Y.-L. Xiong, 2005. Calculation of Organic-Ligand Concentrations for the WIPP Performance-Assessment Baseline Calculations. Sandia National Laboratories, Carlsbad, NM. ERMS 539635.

Clayton, D.J. 2007. Justification of Relative Permeability and Capillary Pressure Model Parameters for Use by BRAGFLO Version 6.0. Sandia National Laboratories, Carlsbad, NM. ERMS 545764.

Clayton, D.J. and E.D. Vugrin. 2007. Justification of Chemistry Parameters for Use by BRAGFLO Version 6.0. Sandia National Laboratories, Carlsbad, NM. ERMS 545611.

Cotsworth, E. 2005. EPA Letter on Conducting the Performance Assessment Baseline Change (PABC) Verification Test. U.S. EPA, Office of Radiation and Indoor Air, Washington, D.C. ERMS 538858.

Deng, H. 2007. MgO Hydration Rate. Sandia National Laboratories, Carlsbad, NM. ERMS 545757.

Dunagan, S. 2007. Parameter Problem Report (PPR), PPR-2007-001 for REFCON:FVW. Sandia National Laboratories, Carlsbad, NM. ERMS 545481.

Garner, J.W. and C.D. Leigh. 2005. Analysis Package for PANEL, CRA-2004 Performance Assessment Baseline Calculation, Revision 0. Sandia National Laboratories, Carlsbad, NM. ERMS 540572.

Gilkey, A.P. 2006. Change Control Form for NUTS version 2.05A (proposed version 2.05C). Sandia National Laboratories, Carlsbad, NM. ERMS 543393.

Gilkey, A.P. 2007. Change Control for PREBRAG, Version 7.00, (Proposed 8.00). Sandia National Laboratories, Carlsbad, NM. ERMS 545263.

Ismail, A.E. 2007a. Parameter Problem Report (PPR), PPR-2007-002 for S\_HALITE, DRZ\_0. Sandia National Laboratories, Carlsbad, NM. ERMS 545713.

Ismail, A.E. 2007b. Revised Porosity Estimates for the DRZ. Sandia National Laboratories, Carlsbad, NM. ERMS 545755.

Kanney, J.F. and C.D. Leigh. 2005. SNL WIPP Analysis Plan AP-122, Revision 0, Analysis Plan for Post CRA PA Baseline Calculation. Sandia National Laboratories, Carlsbad, NM. ERMS 539624.

Kessel, D.S. 2007. FW, PA Parameter Peer Review. Email from R. Patterson to R. Steger. ERMS 547404.

Kirchner, T.B. 2005a. Generation of the LHS Samples for the CRA 2004 PA Baseline Calculations, Revision 0. Sandia National Laboratories, Carlsbad, NM. ERMS 540279.

Kirchner, T.B. 2005b. Sensitivity of Performance Assessment Baseline Calculation Releases to Parameters. Sandia National Laboratories, Carlsbad, NM. ERMS 540767.

Kirkes, G.R. 2007. Evaluation of the Duration of Direct Brine Release in WIPP Performance Assessment, Revision 0. Sandia National Laboratories, Carlsbad, NM. ERMS 545988.

Kirkes, G.R. and C.G. Herrick. 2006. Analysis Plan for the Modification of the Waste Shear Strength Parameter and Direct Brine Release Parameters, AP-131. Sandia National Laboratories, Carlsbad, NM. ERMS 541530.

Leigh, C.D., J.F. Kanney, L.H. Brush, J.W. Garner, G.R. Kirkes, T. Lowry, M.B. Nemer, J.S. Stein, E.D. Vugrin, S. Wagner and T.B. Kirchner. 2005a. 2004 Compliance Recertification Application Performance Assessment Baseline Calculation, Revision 0. Sandia National Laboratories, Carlsbad, NM. ERMS 541521.

Leigh, C.D., J.R. Trone and B. Fox 2005b. TRU Waste Inventory for the 2004 Compliance Recertification Application Performance Assessment Baseline Calculation. Sandia National Laboratories, Carlsbad, NM. ERMS 541118.

Lowry, T. and J. Kanney. 2005. Analysis Report for the CRA-2004 PABC Culebra Flow and Transport Calculations. Sandia National Laboratories, Carlsbad, NM. ERMS 541508.

MacKinnon, R.J. and G. Freeze. 1997a. Summary of EPA-Mandated Performance Assessment Verification Test (Replicate 1) and Comparison With the Compliance Certification Application Calculations, Revision 1. Sandia National Laboratories, Carlsbad, NM. ERMS 422595

MacKinnon, R.J. and G. Freeze. 1997b. Summary of Uncertainty and Sensitivity Analysis Results for the EPA-Mandated Performance Assessment Verification Test, Rev. 1. Sandia National Laboratories, Carlsbad, NM. ERMS 420669.

MacKinnon, R.J. and G. Freeze. 1997c. Supplemental Summary of EPA-Mandated Performance Assessment Verification Test (All Replicates) and Comparison With the Compliance Certification Application Calculations, Revision 1. Sandia National Laboratories, Carlsbad, NM. ERMS 414880.

Nemer, M.B. 2007a. Change Control for BRAGFLO, Version 5.0, (Proposed 6.0). Sandia National Laboratories, Carlsbad, NM. ERMS 544904.

Nemer, M.B. 2007b. Change Control for POSTBRAG, Version 4.00, (Proposed 4.00A). Sandia National Laboratories, Carlsbad, NM. ERMS 545687.

Nemer, M.B. 2007c. Design Document for BRAGFLO Version 6.0. Sandia National Laboratories, Carlsbad, NM. ERMS 545015.

Nemer, M.B. 2007d. Effects of Not Including Emplacement Materials in CPR Inventory on Recent PA Results. Sandia National Laboratories, Carlsbad, NM. ERMS 545689.

Nemer, M.B. 2007e. Software Problem Report (SPR) 07-001 for POSTBRAG, Version 4.00. Sandia National Laboratories, Carlsbad, NM. ERMS 545686.

Nemer, M.B. 2007f. Software Quality Assurance Plan for BRAGFLO Version 6.0. Sandia National Laboratories, Carlsbad, NM. ERMS 545013.

Nemer, M.B. 2007g. User's Manual for BRAGFLO Version 6.0. Sandia National Laboratories, Carlsbad, NM. ERMS 545016.

Nemer, M.B. 2007h. Validation Document for BRAGFLO Version 6.0. Sandia National Laboratories, Carlsbad, NM. ERMS 545018.

Park, B.-Y. and A.E. Ismail. 2007. Analysis Plan for Prediction of the Extent and Permeability of the Disturbed Rock Zone around a WIPP Disposal Room, AP-133, Revision 0. Sandia National Laboratories, Carlsbad, NM. ERMS 545340.

Stoelzel, D.M. and D.G. O'Brien. 1996. Conceptual Model Description of BRAGFLO Direct Brine Release Calculations to Support the Compliance Certification Application (CCA MASS Attachment 16-2). U.S. Department of Energy, Carlsbad, NM. ERMS 239090.

U.S. Congress. 1992. WIPP Land Withdrawal Act, Public Law 102-579, 106 Stat. 4777, 1992; as amended by Public Law 104-201, 110 Stat. 2422, 1996.

U.S. Department of Energy (DOE). 1996. Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot. DOE/CAO-1996-2184, U.S. Department of Energy Waste Isolation Pilot Plant, Carlsbad Area Office, Carlsbad, NM.

DOE. 2004. Title 40 CFR Part 191 Compliance Recertification Application for the Waste Isolation Pilot Plant, DOE/WIPP 2004-3231, 10 vols., US Department of Energy, Carlsbad Field Office, Carlsbad.

DOE/WIPP. 2007. Delaware Basin Monitoring Annual Report. DOE/WIPP-07-2308.

US Environmental Protection Agency (EPA). 1998. 40 CFR 194, Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance with the Disposal Regulations: Certification Decision: Final Rule, Federal Register. Vol. 63, 27354-27406. ERMS 251924.

Vugrin, E.D. 2005. Analysis Package for DRSPALL, CRA 2004 Performance Assessment Baseline Calculation. Sandia National Laboratories, Carlsbad, NM. ERMS 540415.

Vugrin, E.D. and M.B. Nemer. 2007. Analysis Plan for the 2009 Compliance Recertification Application Performance Assessment, AP-132, Revision 0. Sandia National Laboratories, Carlsbad, NM. ERMS 545496.

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