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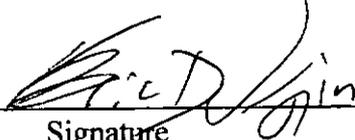
**Sandia National Laboratories  
Waste Isolation Pilot Plant**

**Analysis Plan for the 2009 Compliance Recertification  
Application Performance Assessment**

**Task Number**

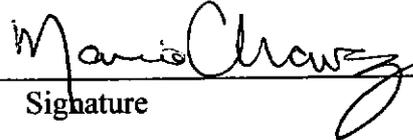
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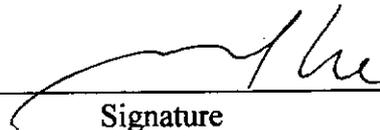
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Author: Eric D. Vugrin (6711)  2/28/07  
Print Signature Date

Author: Martin B. Nemer (6711)  2/28/07  
Print Signature Date

Technical Review: Daniel J. Clayton (6711)  2/28/07  
Print Signature Date

QA Review: Mario J. Chavez (6710)  2/28/07  
Print Signature Date

Management Review: Moo Y. Lee (6711)  2/28/07  
Print Signature Date

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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 performance assessment 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).

Experiments and analyses have continued to further understanding of the repository since the initial certification of the WIPP. Inclusion of the results of these analyses in WIPP PA will result in a more accurate representation of the repository and better predictions of the long term performance of the repository. Subsequent to the completion of the CRA-2004 PA, SNL staff members reviewed WIPP PA conceptual models and parameters with the goal of identifying those that could be improved by implementing results from ongoing repository investigations. Hansen and Stein (2005) identified five components of the repository system that were either not represented in WIPP PA process models or could be implemented in alternative manners that are more consistent with the expected state of the repository. Additionally, Hansen and Stein (2005) made a set of recommendations about how the PA models could be modified to better represent these components. Hansen (2005) reviewed the waste shear strength parameter in the WIPP PA cavings model and concluded that "the values used for this parameter are extraordinarily low and without justification. Examination of the documentation for this parameter shows that there is no connection between the values implemented in WIPP performance assessment and the expected evolution of the underground based on known features, events and processes."

A series of meetings with SNL staff members were held to assess and prioritize PA modifications, and a report (Nemer and Leigh 2006) containing recommended PA changes was created and submitted to the DOE. Nemer and Leigh's (2006) recommendations were further discussed by DOE and SNL staff members, and it was concluded that the following enhancements can and should be implemented at this time:

- 1) Healing of the DRZ should be included in WIPP PA.
- 2) Quantities of brine that are available to travel into waste areas from the DRZ should be re-evaluated. These quantities are a function of DRZ properties including the dimensions (size) and porosity of the DRZ.
- 3) Changes to chemistry models that affect brine saturations in the brine and gas flow model BRAGFLO should be implemented. These changes include magnesium oxide (MgO) hydration and carbonation and steel sulfidation.
- 4) The parameter distribution for waste shear strength should be revised to be more representative of the expected final state of the waste.
- 5) The parameters determining the maximum and minimum duration of a direct brine release should be modified.

The first three modifications were recommended by Hansen and Stein (2005) and impact the Salado flow calculations implemented in the BRAGFLO process model. The fourth change was recommended by Hansen (2005), and the final modification was proposed in internal discussions.

This document details an analysis that will assess the impact of these PA enhancements on the long term performance of the repository. To assess the impact, a full set of PA calculations will be executed. The results of these calculations will be presented in three related forums.

- 1) 40 CFR Part 194.23 requires that all WIPP PA conceptual models be peer reviewed, and, historically, the EPA has required that any "significant" changes to previously peer reviewed models be peer reviewed, as well. Inclusion of DRZ healing represents a significant change to the conceptual model for the DRZ, so portions of this analysis will be presented to a peer review panel.
- 2) Per 40 CFR 194.4, changes to the WIPP PA baseline must be reported to the EPA prior to the implementation or annually in the Annual Change Report, depending on the significance of the change. Thus, the analysis described herein will be submitted to the EPA as part of a planned change request (PCR) currently planned for submittal in March 2008.
- 3) The Land Withdrawal Act (US Congress 1992) requires that the DOE apply for recertification every five years from the first receipt of waste. Thus, the DOE will be required to submit another Compliance Recertification Application in March 2009, and 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.

## 2 APPROACH

This analysis, henceforth referred to as the CRA-2009 PA, seeks to answer the following question: how is the long-term repository performance affected by the inclusion of the five WIPP PA enhancements described in Section 1? To answer this question, a full set of PA calculations will be executed with these PA enhancements, 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 enhancements, 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 five PA enhancements listed in Section 1 primarily affect three WIPP PA process models. DRZ healing, quantities of brine in the DRZ, and the aforementioned chemistry modifications will be included in the WIPP PA brine and gas flow model that is implemented in the numerical code BRAGFLO. Modifying the waste shear strength used for the cavings model will affect cavings volumes calculated by the code CUTTINGS\_S, and changing the direct brine release (DBR) duration parameters used for the direct brine release model may affect DBR volumes calculated by the code BRAGFLO\_DBR<sup>1</sup>. 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.

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<sup>1</sup> The code BRAGFLO 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.

## **2.1 Major Changes Relative to CRA-2004 PABC**

The CRA-2009 PA will contain three groups of major changes from CRA-2004 PABC: 1) modifications to the DRZ conceptualization and chemistry models in the BRAGFLO model; 2) modification of the waste shear strength parameter in the cavings model; and 3) modification of the DBR duration parameters. The following sections describe how these issues were modeled in the CRA-2004 PABC and how they will be modified for the CRA-2009 PA.

### **2.1.1 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 consolidation and closure, gas generation, brine consumption, and inter-bed fracturing in response to gas pressure. Several of the PA enhancements listed in Section 1 affect the BRAGFLO code, and these enhancements can be grouped into three categories:

- 1) Modifications affecting the DRZ;
- 2) Incorporating additional geochemical reactions that affect the calculation of the water budget and brine saturation levels; and
- 3) Modifications to improve performance of the code.

#### **2.1.1.1 DRZ Modifications**

The DRZ, as modeled in WIPP PA, is an important feature of the repository system because its properties affect both the quantity of brine and its ability to enter the waste areas. The DRZ has been re-examined in considerable detail since operations initiated, and Hansen (2003) concluded that WIPP PA overestimates the extent and permeability of the DRZ for the majority of the 10,000 year regulatory time period.

The CRA-2009 will make the following changes to how the DRZ is modeled in the BRAGFLO process model:

- 1) The size and the extent of the DRZ may be changed; and
- 2) The permeability of the DRZ may be modified to include DRZ healing.
- 3) The porosity of the DRZ will be examined and may be modified.

#### **DRZ Extent and Healing**

For the CRA-2004 PABC, the DRZ extended 11.95 m above and 2.23 m below the waste area, panel closures, operations area, and experimental area in the two-dimensional, semi-vertically oriented BRAGFLO computational grid (Figure 1), that represents the vicinity of a waste panel to the surrounding halite, marker beds, and other geologic formations. The dimensions of the DRZ were held constant in all CRA-2004 PABC simulations.

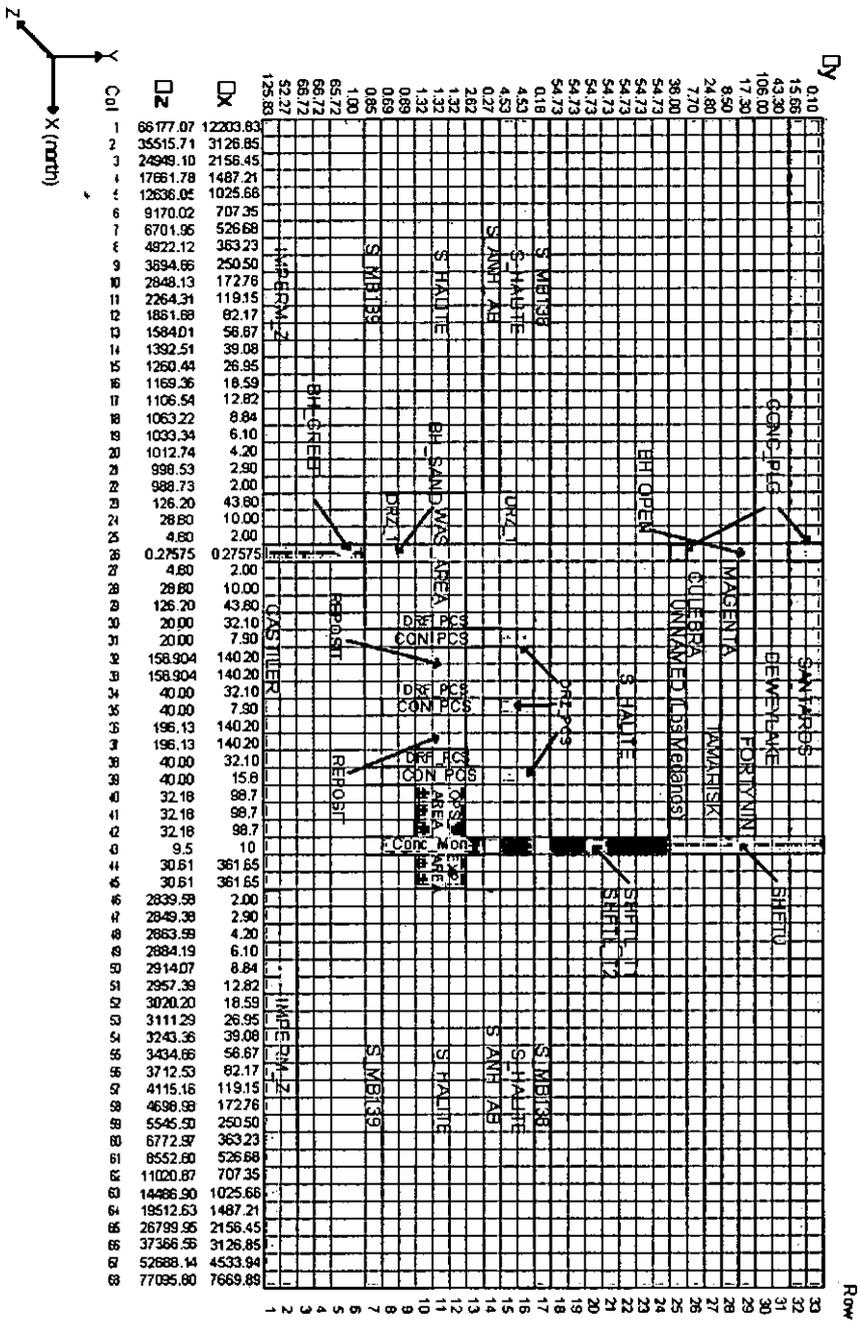


Figure 1 CRA-2004 PABC BRACFLO Computational Grid  
 The yellow grid cells labeled "DRZ\_1" are the locations where the DRZ is modeled in BRACFLO simulations.

Information Only

Two materials were used to represent the DRZ at different times during BRAGFLO simulations. The material DRZ\_0 represented the properties of the DRZ for the five years prior to the closure of the WIPP facility (years -5 to 0), and the material DRZ\_1 represented the properties of the DRZ after closure during the 10,000 year regulatory time period (years 0 to 10,000). For the CRA-2004 PABC, the DRZ was assigned a permeability of  $10^{-17} \text{ m}^2$  (in all directions) for years -5 to 0, and after closure of the repository, the DRZ was assigned a permeability (in all directions) that was randomly sampled from the loguniform distribution on  $[10^{-12.5}, 10^{-19.4}]$  (Table 1). For each BRAGFLO simulation, the permeability was held constant for years 0 to 10,000.

**Table 1 DRZ Permeability and Initial Brine Saturation Parameters used in the CRA-2004 PABC**

Property	Description	Units	Material	Parameter Type	Value(s)
PRMX_LOG	Log <sub>10</sub> of the intrinsic permeability in the X-direction <sup>1</sup>	Log <sub>10</sub> (m <sup>2</sup> )	DRZ_0	Constant	-17.0
			DRZ_1	Uniform Distribution	[-12.5,-19.4]
SAT_IBRN	Initial brine saturation	Unitless	DRZ_0	Constant	1.00

<sup>A</sup> For the CRA-2004 PABC, the parameter DRZ\_1:PRMX\_LOG was sampled once for each vector, and the sampled values were assigned to the properties DRZ\_1:PRMY\_LOG and DRZ\_1:PRMZ\_LOG.

*Analysis Plan for Numerical Prediction of the Disturbed Rock Zone with Permeability Around WIPP Disposal Room, AP-133* (Park and Ismail 2007) is an analysis plan that was developed to reevaluate the extent of the DRZ and the properties of the DRZ after significant healing has occurred. This analysis will incorporate data from ultrasonic wave speed measurements that characterize the DRZ (Holcomb and Hardy 2001) with modeling results from the quasistatic, large-deformation finite element code SANTOS to assess the extent of the DRZ. The AP-133 analysis will also determine the length of time required for the DRZ to finish healing, i.e. the time required for the DRZ to reach an equilibrium or steady-state. (This time is denoted by  $t_{SS}$  in this document.) AP-133 introduces a new material, DRZ\_2, that will represent the DRZ for all times after  $t_{SS}$ . Most of the properties associated with the material DRZ\_2 will have identical values to the corresponding DRZ\_1 properties, but pending the results of the analysis detailed in AP-133, the DRZ\_2 permeability may differ from the DRZ\_1 permeability.

The CRA-2009 PA will use the results of the AP-133 in the following manner:

- 1) If the AP-133 analysis concludes that the dimensions of the DRZ are significantly different than the dimensions used in the current BRAGFLO computational grid, the CRA-2009 BRAGFLO calculations will use the dimensions recommended by the AP-133 analysis. Otherwise, the CRA-2009 PA will use the same size DRZ as was used in the CRA-2004 PABC.
- 2) During the time period -5 to 0 years, the DRZ will be modeled with the material DRZ\_0. For years 0 to  $t_{SS}$ , the DRZ will be modeled with the

material DRZ\_1. The CRA-2009 PA will use the time  $t_{SS}$  determined by the AP-133 analysis. For the remainder of the 10,000 year regulatory time period, the DRZ will be modeled with the material DRZ\_2. The DRZ\_2 property values will be determined by the AP-133 analysis.

- 3) The permeability of the DRZ will smoothly transition from the DRZ\_1 value to the DRZ\_2 value between year 0 and year  $t_{SS}$ . The algorithm for calculating the changing permeability is discussed in WIPP PA (2006a, 2006b, 2006c).

### **DRZ Porosity**

In BRAGFLO calculations, the porosity of the DRZ is used to determine the quantity of brine stored in the DRZ. For the CRA-2004 PABC, the porosity of intact Salado halite (S\_HALITE:POROSITY) was sampled from the range [0.001,0.03], and the porosity of the DRZ materials (DRZ\_0 and DRZ\_1) was determined by adding 0.0029 to the sampled halite porosity. Thus, the DRZ porosity was effectively sampled on the range [0.0039,0.0329], and the DRZ and halite porosities were directly correlated with a correlation factor of 1.

The basis for determining the DRZ\_0 and DRZ\_1 porosity parameter distributions will be reviewed to assess if these parameters should be modified. Pending the outcome of the review, these parameters may be modified or additional parameters may be created, the CRA-2009 PA will use the revised parameters.

#### **2.1.1.2 Modifications to the Water Budget Calculation**

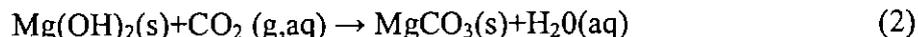
The CRA-2004 PABC did not include MgO hydration and carbonation and iron sulfidation. These reactions have the potential to affect the water budget that BRAGFLO uses to calculate brine saturations in the waste areas, so the CRA-2009 PA will include these chemical reactions.

#### **MgO Hydration**

Brush and Roselle (2006) indicate that MgO hydrates rapidly to form brucite when water is available (Eq. 1), and in this reaction, water is removed from the system.



However, when brucite carbonates to form magnesite, water is released (Eq. 2).



These reactions will be included to calculate the water budget that determines brine saturation in the CRA-2009 BRAGFLO simulations. In the event that CO<sub>2</sub> production is occurring but brucite is not available in BRAGFLO simulations, MgO will be converted directly to magnesite. This direct conversion is included to account for humid conditions at very low saturation levels.

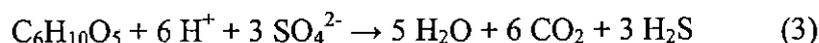
Inclusion of the MgO hydration and carbonation reactions in the CRA-2009 PA requires the creation of two new parameters (Table 2). Experiments have been conducted in accordance with TP 00-07, *Experimental study of WIPP Engineered Barrier MgO at Sandia National Laboratories Carlsbad Facility* (Snider et al. 2004) to determine the rates of MgO hydration, and the results of these experiments will be used to define the parameters WAS\_AREA:BRUCITEI and WAS\_AREA:BRUCITEH. These parameters will represent the rate of MgO hydration in inundated and humid conditions, respectively. MgO carbonation (Eq. 2) will be assumed to proceed at the same rate as CO<sub>2</sub> production rate. This approach is consistent with the preliminary results (Nowak and Clayton 2007) of an analysis being conducted under AP-108, *Analysis of MgO Hydration and Carbonation Test Results* (Nowak 2003). (The parameters WAS\_AREA:GRATMICH and WAS\_AREA:GRATMICI represent CO<sub>2</sub> production rates for humid and inundated conditions, respectively.)

Table 2 MgO Hydration Parameters to be Created for the CRA-2009 PA

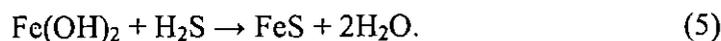
Material Name	Property Name	Parameter Description
WAS_AREA	BRUCITEI	Rate of MgO hydration under inundated conditions
WAS_AREA	BRUCITEH	Rate of MgO hydration under humid conditions

### Iron Sulfidation

When cellulose, plastic, and rubber (CPR) materials are degraded by sulfate reduction, hydrogen sulfide (H<sub>2</sub>S) is produced (Eq. 3).



The H<sub>2</sub>S is assumed to react immediately on time scales of interest with iron or iron hydroxide to form FeS according to Eqs. 4 and 5.



Reactions 4 and 5 will be included to calculate the water budget that determines brine saturation in the CRA-2009 BRAGFLO simulations. Because reaction 5 returns water to the waste filled areas, the CRA-2009 will conservatively assume that reaction 5 kinetically dominates reaction 4 if iron hydroxide is available. If iron hydroxide is not available, it will be assumed that reaction 4 occurs. In both cases the rate of iron sulfidation will be equal to the CO<sub>2</sub> production rate times a factor,  $\gamma$ . This factor represents the ratio of moles of H<sub>2</sub>S produced to the moles of organic carbon consumed when all of the organic carbon in the emplaced CPR materials is consumed by microbes. Since WIPP PA assumes that denitrification and sulfate reduction are

the only mechanisms for degradation of CPR materials and H<sub>2</sub>S is not a byproduct of denitrification, this factor,  $y$ , is calculated according to Eq. 6.

$$y = (1 - F_D) \times 0.5 \quad (6)$$

$F_D$  denotes the fraction of the moles of organic carbon in CPR materials that could be consumed by denitrification, and the 0.5 factor is included in Eq. 6 since 0.5 moles of H<sub>2</sub>S are produced for every mole of CO<sub>2</sub> during sulfate reduction.

### 2.1.1.3 Code Version

The CRA-2004 PABC used BRAGFLO version 5.0 for Salado flow calculations. BRAGFLO version 6.0 will be used for the CRA-2009 PA. BRAGFLO version 5.0 does not have the capability to include the chemistry reactions discussed in Section 2.1.1.2, so BRAGFLO version 6.0 is being developed to implement these enhancements. 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 WIPP PA (2006a, 2006b, 2006c).

### 2.1.2 Waste Shear Strength

WIPP PA includes scenarios in which an exploratory gas or oil borehole intersects a waste room of the repository. It is hypothesized that the circulating drilling fluids will apply shearing stresses to the borehole wall, causing erosion within the borehole. The eroded portion of the borehole is called cavings. Although a number of factors affect erosion within a borehole (Broc 1982), the most important factor is believed to be the fluid shear stress on the borehole wall (i.e., the shearing force per unit area, (kg m/s<sup>2</sup>/m<sup>2</sup>)) resulting from circulating drilling fluids (Darley 1969, Walker and Holman 1971). In particular, the borehole diameter is assumed to grow until the shear stress on the borehole wall is equal to the shear strength of the waste (i.e., the limiting shear stress below which the erosion of the waste ceases).

WIPP PA uses the parameter BOREHOLE:TAUFAIL to represent the shear strength of the waste, and Table 3 lists the properties of the parameter distribution that was used in the CRA-2004 PABC. *Analysis Plan for the Modification of the Waste Shear Strength Parameter and Direct Brine Release Parameters, AP-131* (Kirkes and Herrick 2006) describes an analysis that is being conducted to revise the parameter distribution for the parameter BOREHOLE:TAUFAIL. If the AP-131 analysis recommends changes to the BOREHOLE:TAUFAIL parameter, the CRA-2009 PA will use the new parameter distribution.

**Table 3 Waste Shear Strength Parameter for the CRA-2004 PABC**

Name	Description	Units	Parameter Type	Range
BOREHOLE:TAUFAIL	Effective waste shear strength	Pa	Lognormal Distribution	[0.05,77]

**2.1.3 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 direct brine releases (DBRs).

The duration of a DBR event is constrained by the parameters BLOWOUT:MINFLOW and BLOWOUT:MAXFLOW. BLOWOUT:MINFLOW represents the minimum DBR duration time, and 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 (Table 4). *Analysis Plan for the Modification of the Waste Shear Strength Parameter and Direct brine Release Parameters, AP-131* (Kirkes and Herrick 2006) describes an analysis that is being conducted to revise the values of the parameters BLOWOUT:MINFLOW and BLOWOUT:MAXFLOW. If the AP-131 analysis concludes that these parameters should be modified, the CRA-2009 PA will use the new DBR duration parameters.

**Table 4 DBR Duration Parameters for the CRA-2004 PABC**

Name	Description	Units	Parameter Type	Value (seconds)
BLOWOUT:MINFLOW	Minimum DBR duration	Seconds	Constant	2.592E+5
BLOWOUT:MAXFLOW	Maximum DBR Duration	Seconds	Constant	9.504E+5

**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 will be 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 features, events, and processes (FEPs) baseline must be conducted according to SP 9-4, *Performing FEPs Impact Assessment for Planned or Unplanned Changes*, 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 as defined in SP 9-4.

### 2.4 Inventory

Leigh et al. (2005b) gives a comprehensive description of the projected inventory that was used for the CRA-2004 PABC. The CRA-2004 PABC inventory is a part of the current EPA-approved PA baseline and it is the most recent inventory. The CRA-2009 will use the this inventory with one set of modifications.

The CRA-2004 PABC included CPR materials in the waste and container (packaging) materials (Table 5), but the CPR contents in emplacement materials were erroneously omitted from the CRA-2004 PABC (Nemer 2007). To correct this omission, six new parameters representing the density of CPR materials in emplacement materials will be created and used in the CRA-2009 PA. Table 6 lists the names and descriptions of these container parameters. Four additional parameters will be created and represent the density of cellulose and rubber materials in container (packaging) materials (Table 6). The addition of these parameters is done solely for book-keeping purposes since packaging materials, do not contain cellulose or rubber materials. The CRA-2009 PA will use the parameters in Table 6, in addition to the CRA-2004 PABC CPR parameters.

Table 5 CRA-2004 PABC Cellulose, Plastic and Rubber Parameters

PROPERTY:MATERIAL	Description
WAS AREA: DCELLCHW	Average density of cellulose in CH waste materials
WAS AREA: DCELLRHW	Average density of cellulose in RH waste materials
WAS AREA: DRUBBCHW	Average density of rubber in CH waste materials
WAS AREA: DRUBBRHW	Average density of rubber in RH waste materials
WAS AREA: DPLASCHW	Average density of plastic in CH waste materials
WAS AREA: DPLSCCHW	Average density of plastic in CH waste container (packaging) materials
WAS AREA: DPLASRHW	Average density of plastic in RH waste materials
WAS AREA: DPLSCRHW	Average density of plastic in RH waste container (packaging) materials

**Table 6 Cellulose, Plastic and Rubber Parameters to be Created for the CRA-2009 PA**

<b>PROPERTY:MATERIAL</b>	<b>Description</b>
WAS_AREA:DPLSECHW	Average density of plastic in CH waste emplacement materials
WAS_AREA:DPLSERHW	Average density of plastic in RH waste emplacement materials
WAS_AREA:DCELECHW	Average density of cellulose in CH waste emplacement materials
WAS_AREA:DCELERHW	Average density of cellulose in RH waste emplacement materials
WAS_AREA:DRUBECHW	Average density of rubber in CH waste emplacement materials
WAS_AREA:DRUBERHW	Average density of rubber in RH waste emplacement materials
WAS_AREA:DCELCCHW	Average density of cellulose in CH waste container materials
WAS_AREA:DCELCRHW	Average density of cellulose in RH waste container materials
WAS_AREA:DRUBCCHW	Average density of rubber in CH waste container materials
WAS_AREA:DRUBCRHW	Average density of rubber in RH waste container materials

## 2.5 Parameters

Table 7 lists the parameters that are being created for the CRA-2009 PA or were created after the CRA-2004 PABC and were not used in that assessment, and Table 8 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).

Note that the CRA-2009 PA will use a different value for the parameter REFCON:FVW because that parameter was modified after the CRA-2004 PABC to correct an error in how it was calculated. *Parameter Problem Report PPR 2007-01* discusses the error and the minor impact that it had on spillings and cuttings release calculations by the code CCDFGF.

In the WIPP PA parameter database, the DRZ\_1 material is described as “disturbed rock zone: time period 0 to 10,000 years.” This description will no longer be appropriate since the DRZ\_1 material will not be used to describe the DRZ for the full 10,000 year regulatory time period. Rather, the DRZ\_1 material description in the parameter database will be changed to the following: “disturbed rock zone during the time period that begins with facility closure (0 years) and ends when DRZ healing is complete.”

Table 7 CRA-2009 PA Parameters Not Used in the CRA-2004 PABC .

Material	Property	Description	Application	Guiding Document
DRZ_2	CAP_MOD	Model number, capillary pressure model	BRAGFLO	AP-133
	COMP_RCK	Bulk compressibility	BRAGFLO	AP-133
	KPT	Flag for permeability determined threshold	BRAGFLO	AP-133
	PC_MAX	Maximum capillary pressure	BRAGFLO	AP-133
	PCT_A	Threshold pressure constant parameter	BRAGFLO	AP-133
	PCT_EXP	Threshold pressure exponential parameter	BRAGFLO	AP-133
	PO_MIN	Minimum brine pressure	BRAGFLO	AP-133
	PORE_DIS	Pore distribution parameter	BRAGFLO	AP-133
	POROSITY	Porosity	BRAGFLO	AP-133
	PRMX_LOG	Log of permeability in the x-direction	BRAGFLO	AP-133
	PRMY_LOG	Log of permeability in the y-direction	BRAGFLO	AP-133
	PRMZ_LOG	Log of permeability in the z-direction	BRAGFLO	AP-133
	RELP_MOD	Relative permeability model number	BRAGFLO	AP-133
	SAT_IBRN	Initial brine saturation	BRAGFLO	AP-133
	SAT_RBRN	Residual brine saturation	BRAGFLO	AP-133
	SAT_RGAS	Residual gas saturation	BRAGFLO	AP-133
	DPHI_MAX	Constant incremental increase in porosity relative to intact salt	BRAGFLO	AP-133
	IFRX	Index for fracture permeability enhancement in the x-direction	BRAGFLO	AP-133
	IFRY	Index for fracture permeability enhancement in the y-direction	BRAGFLO	AP-133
	IFRZ	Index for fracture permeability enhancement in the z-direction	BRAGFLO	AP-133
PF_DELTA	Incremental pressure for full fracture development	BRAGFLO	AP-133	
PI_DELTA	Fracture initiation pressure increment	BRAGFLO	AP-133	
WAS_AREA	DPLSECHW	Average density of plastic in CH waste emplacement materials	BRAGFLO	Nemer 2007
	DPLSERHW	Average density of plastic in RH waste emplacement materials	BRAGFLO	Nemer 2007
	DCELECHW	Average density of cellulose in CH waste emplacement materials	BRAGFLO	Nemer 2007
	DCELERHW	Average density of cellulose in RH waste emplacement materials	BRAGFLO	Nemer 2007
	DRUBECHW	Average density of rubber in CH waste emplacement materials	BRAGFLO	Nemer 2007
	DRUBERHW	Average density of rubber in RH waste emplacement materials	BRAGFLO	Nemer 2007

Material	Property	Description	Application	Guiding Document
	DCELCCHW	Average density of cellulose in CH waste container materials	BRAGFLO	Nemer 2007
	DCELCRHW	Average density of cellulose in RH waste container materials	BRAGFLO	Nemer 2007
	DRUBCCHW	Average density of rubber in CH waste container materials	BRAGFLO	Nemer 2007
	DRUBCRHW	Average density of rubber in RH waste container materials	BRAGFLO	Nemer 2007
	BRUCITEI	Rate of MgO hydration under inundated conditions	BRAGFLO	Nemer 2007
	BRUCITEH	Rate of MgO hydration under humid conditions	BRAGFLO	Nemer 2007

Table 8 CRA-2009 PA Parameters Modified from CRA-2004 PABC Values

Material	Property	Description	Application	Guiding Document
BLOWOUT	MINFLOW	Minimum blowout flow	BRAGFLO_DBR	AP-131
	MAXFLOW	Maximum blowout flow	BRAGFLO_DBR	AP-131
BOREHOLE	TAUFAIL	Effective waste shear strength for erosion	CUTTINGS_S	AP-131
REFCON	FVW	Fraction of Repository Volume Occupied By Waste In CCDFGF Model	CCDFGF	PPR 2007-01
DRZ_0	POROSITY	Effective Porosity	BRAGFLO	AP-132
DRZ_1	POROSITY	Effective Porosity	BRAGFLO	AP-132

## 2.6 Calculations

### 2.6.1 Parameter Sampling: LHS

Three replicates of 100 vectors will be created using the Latin Hypercube sampling code LHS, and the random seed and parameter ordering from the CRA-2004 PABC will be preserved. 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. If any of the parameters being developed for the CRA-2009 PA (Table 7) are assigned probability distributions, those parameters will be sampled, as well.

It is expected that the AP-133 analysis will recommend a probability distribution for the parameter DRZ\_2:PRMX\_LOG, the log of the permeability (in the X-direction) of the DRZ after healing has taken place, so this parameter will likely be sampled by the code LHS. The CRA-2009 PA will not impose a correlation between the DRZ\_1 and DRZ\_2 parameters, so if the DRZ\_1 and DRZ\_2 permeability parameter ranges overlap, it is possible that LHS may sample a higher DRZ\_2 permeability value than DRZ\_1 permeability value for a single vector. This combination of parameters would imply that the permeability of the DRZ increases after healing, a physically unrealistic scenario. Hence, a utility will be developed that ensures the sampled DRZ\_1 permeability value for a vector is higher than the sampled DRZ\_2 permeability value for that same vector. This utility will post-process the LHS output file and create an output file that will be input into the code POSTLHS.

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 consolidation and closure, gas generation, brine consumption, and inter-bed fracturing in response to gas pressure. BRAGFLO version 6.0 will be used for the Salado flow calculations. A complete suite of calculations will be run for the CRA-2004 PABC: 3 replicates, 100 vectors per replicate, and 6 scenarios (Table 9) per vector.

Table 9 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

BRAGFLO calculations will be conducted as outlined in AP-122 (Kanney and Leigh 2005) with the following exceptions:

- 1) The BRAGFLO computational grid may be modified to incorporate new DRZ dimensions. The decision to modify the grid will be based upon the results of the AP-133 analysis.
- 2) DRZ healing will be modeled;
- 3) DRZ porosity parameters may be modified;
- 4) MgO hydration and carbonation will be included when assessing the water budget; and
- 5) Iron sulfidation will be included when assessing the water budget.

These modifications and their implementations are detailed in Sections 2.1.1.1 and 2.1.1.2. 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.

Additionally, BRAGFLO calculations will be performed with only the DRZ modifications (Section 2.1.1.1) and not the additional chemistry reactions that affect the water budget (Section 2.1.1.2). This intermediate calculation will allow analysts to isolate the impact of the DRZ modifications. This step will include calculations for the undisturbed scenario (S1) and two disturbed scenarios (S3 and S5), in which a single drilling intrusion takes place at 1,000 years after the closure of the repository. In the S3 scenario, a borehole penetrates through the repository into a brine reservoir into a pressurized Castile brine pocket; in the S5 scenario, the borehole stops at the repository. These three scenarios are sufficient to determine the effects on the output variables of the DRZ modifications. The S2 and S4 scenarios repeat the S3 and S5 scenarios, but place the drilling intrusion at 350 years after repository closure. The S6 scenario is a combination of the S3 and S5 scenarios in which two drilling intrusions occur in the same panel, with the second borehole penetrating a brine pocket beneath the repository.

#### *2.6.3 Actinide Mobilization: PANEL*

The PANEL code calculates the quantities of actinides mobilized by colloids and as dissolved species in WIPP brines. 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 are not affected by any of the PA enhancements or parameter changes discussed in Sections 2.1 and 2.5, so actinide mobilization calculations by PANEL from the CRA-2004 PABC will be used for the CRA-2009 PA. 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 (WIPP PA 2006d), so it was modified. NUTS version 2.05C will be used for the CRA-2009 PA.

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 enhancements or parameter changes discussed in Sections 2.1 and 2.5. 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**

Because spallings volumes from a single borehole intrusion are calculated by DRSPALL at initial repository pressures of 10, 12, 14, and 14.8 MPa, implementation of the PA enhancements and parameter changes discussed in Sections 2.1 and 2.5 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. If the AP-131 (Kirkes and Herrick 2006) analysis recommends a new parameter distribution for the waste shear strength (BOREHOLE:TAUFAIL) in the cavings model, the CRA-2009 cuttings and cavings calculation will use the new recommended parameter distribution. With the exception of that parameter, cuttings and cavings calculations will be implemented according to the procedure outlined in AP-122 (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 spillings volume for each scenario, time, location, and vector combination by interpolating the CRA-2004 PABC DRSPALL results using the initial pressure from BRAGFLO (WIPP PA 2004).

### 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 necessary, the DBR calculations will use the BRAGFLO\_DBR parameters that were modified or created after the CRA-2004 PABC (Table 7 and Table 8). These parameters include the DBR duration parameters (BLOWOUT:MAXFLOW and BLOWOUT:MINFLOW) that may be revised, pending the outcome of the AP-131 analysis.
- 2) Instead of BRAGFLO version 5.0, BRAGFLO version 6.0 will be used for the DBR calculations.

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 10).

**Table 10 Direct Brine Release Intrusion times**

DBR Scenario	Intrusion Times (years)
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 enhancements will be implemented in the BRAGFLO calculations, additional sensitivity analyses may 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 11.

**Table 11 Task List and Estimated Schedule for the CRA-2009 PA**

Task	Description	AP/SP/ NP	Approximate Completion Date	Responsible Individual(s)
1	Parameters			
1a	DBR Duration Analysis	AP-131	2/28/07	Kirkes
1b	Waste Shear Strength Analysis	AP-131	2/22/07	Herrick
1c	DRZ Analysis	AP-133, AP-132	3/27/07	Park, Nemer, & Herrick
1d	MgO Hydration Rate Calculation	AP-122	3/22/07	Deng
1e	Parameter Entry	SP 9-5, NP 9-2		Long
2	Code Modifications			
2a	PREBRAG	NP 19-1	3/9/07	Gilkey
2b	BRAGFLO	NP 19-1	3/20/07	Clayton
3	FEPS Re-assessment	SP 9-4		Kirkes
4	Code Run Environment Preparation			
4a	Libraries Update	AP-132	4/6/07	Long
4b	Run Control Script Update	AP-132	4/6/07	Long
5	Calculations			
5a	Parameter Sampling: LHS	AP-132	4/6/07	Long
5b	Salado Flow: BRAGFLO	AP-132	4/20/07	Long
5c	Salado Transport: NUTS & PANEL	AP-132	5/10/07	Long
5d	Cuttings & Cavings: CUTTINGS_S	AP-132	4/23/07	Long
5e	Direct Brine Releases: BRAGFLO_DBR	AP-132	4/27/07	Long
5f	CCDF Construction: CCDFGF	AP-132	5/15/07	Long
5g	Sensitivity Analysis: STEPWISE	AP-132	5/22/07	Long
6	Analysis & Documentation			
6a	Parameter Sampling: LHS	AP-132	8/28/07	Kirchner
6b	Salado Flow: BRAGFLO	AP-132	9/4/07	Nemer & Clayton
6c	Salado Transport: NUTS & PANEL	AP-132	8/28/07	Garner & Ismail
6d	Cuttings & Cavings: CUTTINGS_S	AP-132	8/28/07	Riggins & Herrick
6e	Direct Brine Releases: BRAGFLO_DBR	AP-132	8/28/07	Clayton & Nemer
6f	CCDF Construction: CCDFGF	AP-132	8/28/07	Dunagan
6g	Sensitivity Analysis: STEPWISE	AP-132	8/28/07	Kirchner
6h	Run Control Document	AP-132	8/28/07	Long
6i	Summary Report	AP-132	9/11/07	Vugrin

#### 4 SOFTWARE

The major WIPP PA codes to be used for this analysis are listed in Table 12. These codes will be executed on the WIPP PA Alpha Cluster, which is described in Table 13. Additionally, commercial off-the-shelf (COTS) software, 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 12 Codes to be Used for the CRA-2009 PA

Code	Version	Build Date	Executable
ALGEBRACDB	2.35	31-JAN-1996	ALGEBRACDB PA96.EXE
BRAGFLO <sup>(1)</sup>	6.00		
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	4.00	6-FEB-1996	POSTBRAG PA96.EXE
POSTLHS	4.07A	25-APR-2005	POSTLHS QA0407A.EXE
PREBRAG <sup>(1)</sup>	8.00		
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

<sup>(1)</sup> Build date and executable name are not listed because the code development is in progress.

Table 13 WIPP PA Alpha Cluster

Node	Hardware Type	CPU	Operating System
CCR	HP AlphaServer ES45 Model 2	Alpha EV68	Open VMS 8.2
TDN	HP AlphaServer ES45 Model 2B	Alpha EV68	Open VMS 8.2
BTO	HP AlphaServer ES40	Alpha EV68	Open VMS 8.2
CSN	HP AlphaServer ES40	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

None.

## 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*.

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