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SANDIA NATIONAL LABORATORIES
WASTE ISOLATION PILOT PLANT

AP-164

Analysis Plan for the 2014 WIPP Compliance Recertification Application Performance Assessment

Task 1.2.5

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1 Introduction and Objectives

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) 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 potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. The models used in PA are maintained and updated with new information as part of an ongoing process. Improved information regarding important WIPP features, events, and processes typically results in refinements and modifications to PA models and the parameters used in them. Planned changes to the repository and/or the components therein also result in updates to WIPP PA models. WIPP PA models are used to support the repository recertification process that occurs at five-year intervals following the receipt of the first waste shipment at the site in 1999.

PA calculations were included in the 1996 Compliance Certification Application (CCA) (U.S. DOE 1996), and in a subsequent Performance Assessment Verification Test (PAVT) (MacKinnon and Freeze 1997a, 1997b and 1997c). Based in part on the CCA and PAVT PA calculations, the EPA certified that the WIPP met the regulatory containment criteria. The facility was approved for disposal of transuranic waste in May 1998 (U.S. EPA 1998). PA calculations were an integral part of the 2004 Compliance Recertification Application (CRA-2004) (U.S. DOE 2004). During their review of the CRA-2004, the EPA requested an additional PA calculation, referred to as the CRA-2004 Performance Assessment Baseline Calculation (PABC) (Leigh et al. 2005), be conducted with modified assumptions and parameter values (Cotsworth 2005). Following review of the CRA-2004 and the CRA-2004 PABC, the EPA recertified the WIPP in March 2006 (U.S. EPA 2006).

PA calculations were completed for the second WIPP recertification and documented in the 2009 Compliance Recertification Application (CRA-2009). The CRA-2009 PA resulted from continued review of the CRA-2004 PABC, including a number of technical changes and corrections, as well as updates to parameters and improvements to the PA computer codes (Clayton et al. 2008). To incorporate additional information which was received after the CRA-2009 PA was completed, but before the submittal of the CRA-2009, the EPA requested an additional PA calculation, referred to as the 2009 Compliance Recertification Application Performance Assessment Baseline Calculation (PABC-2009) (Clayton et al. 2010), be undertaken which included updated information (Cotsworth 2009). Following the completion and submission of the PABC-2009, the WIPP was recertified in 2010 (U.S. EPA 2010).

The Land Withdrawal Act (U.S. Congress 1992) requires that the DOE apply for WIPP recertification every five years following the initial 1999 waste shipment. The results of the analysis described herein will be included in the 2014 Compliance Recertification Application (CRA-2014) to demonstrate regulatory compliance with the containment requirements according

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to the Certification Criteria in Title 40 CFR Part 194. This document details how SNL will conduct the compliance decision analysis for the CRA-2014 PA. Potential regulatory compliance impacts resulting from changes since the PABC-2009 will be determined by way of a comparison of CRA-2014 PA release probabilities to those calculated in the PABC-2009.

2 Approach

The CRA-2014 PA analysis will be used to demonstrate compliance with the containment requirements according to the Certification Criteria in Title 40 CFR paragraph 194. PA calculations will be executed that include changes occurring since the PABC-2009 analysis, and results of these calculations will be compared to PABC-2009 results. As regulatory compliance impacts will be assessed via a direct comparison to the PABC-2009, the CRA-2014 PA is designed to reproduce the PABC-2009 implementation where possible. The CRA-2014 PA will examine all aspects of repository performance that are potentially impacted by changes occurring since the PABC-2009.

The approach used for the CRA-2014 PA will be very similar to that used for the PABC-2009 (Clayton 2009). The CRA-2014 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 the 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 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-2014 PA will be implemented with particular attention given to how the CRA-2014 PA implementation will differ from that of the PABC-2009.

2.1 *Changes since the PABC-2009*

Several changes will be incorporated in the CRA-2014 PA relative to the PABC-2009. The modifications included in the CRA-2014 PA include repository planned changes, parameter updates, and refinements to PA implementation. More specifically, changes included in the CRA-2014 PA will include the following:

- Replacement of the "Option D" WIPP panel closure with a newly designed Run-of-Mine Panel Closure System (ROMPCS).
- Inclusion of an additional mined region in the repository north end.
- An update to the probability that a drilling intrusion into a repository excavated region will result in a pressurized brine encounter.
- Refinement to the corrosion rate of steel.

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- Refinement to the effective shear strength of WIPP waste.
- Updates to drilling rate and plugging pattern parameters.
- Updates to WIPP waste inventory parameters.
- Calculation of radionuclide concentration in brine as a function of the actual brine volume present in the waste panel.
- Updates to radionuclide solubilities and their associated uncertainty.
- Implementation of a more detailed repository water balance that includes MgO hydration.
- Parameter corrections.

These changes are discussed in more detail in the sections that follow. It is intended that all modifications to be included in the CRA-2014 PA are captured in the sections that follow. Additional unforeseen changes, if they become necessary, will be discussed in the appropriate CRA-2014 PA analysis package, and also fall under the scope of AP-164.

2.1.1 Replacement of Option D with ROMPCS

WIPP waste panel closures comprise a feature of the repository that has been represented in WIPP PA regulatory compliance demonstration since the CCA of 1996. The 1998 rulemaking that certified WIPP to receive TRU waste required DOE to implement the Option D panel closure system (PCS) at the WIPP. The Option D PCS consists of three primary components, namely, a concrete explosion isolation wall, an open drift section, and a concrete monolith. Following the selection of the Option D panel closure design in 1998, the DOE has reassessed the engineering of the panel closure and established a revised design which is simpler, easier to construct, and equally effective at performing its operational-period isolating function. The DOE has submitted a planned change request (PCR) to the EPA requesting that EPA modify Condition 1 of the Final Certification Rulemaking for 40 CFR Part 194 (U. S. EPA, 1998) for the WIPP, and that a revised panel closure design be approved for use in all panels (U.S. DOE, 2011a). The revised panel closure design, denoted as the ROMPCS, is comprised of 100 feet of run-of-mine (ROM) salt with barriers at each end. The ROM salt is generated from ongoing mining operations at the WIPP while the barriers consist of ventilation bulkheads, similar to those currently used in the panels as room closures. A PA named the PCS-2012 was executed to quantify WIPP repository performance impacts associated with the replacement of the approved Option D PCS design with the ROMPCS. It was found in the PCS-2012 PA (Camphouse et al. 2012b) that implementation of the ROMPCS design does not result in WIPP non-compliance with the containment requirements of 40 CFR Part 191, and that long-term WIPP performance with the ROMPCS design is similar to that seen with Option D.

ROMPCS properties in the PCS-2012 PA were based on three time periods (Camphouse et al. 2012a). Specifically, the ROM salt comprising the ROMPCS was represented by three materials, denoted as PCS_T1 for the first 100 years after facility closure, PCS_T2 from 100 to 200 years, and PCS_T3 for 200 to 10,000 years. For the first 200 years post-closure, the disturbed rock zone (DRZ) above and below the ROMPCS maintained the same properties as specified to the DRZ surrounding the disposal rooms (PA material DRZ_1). After 200 years, the DRZ above and below the ROMPCS was modeled as having healed, and was represented by material DRZ_PCS. Materials DRZ_1 and DRZ_PCS had the same properties in the PCS-2012 PA as were assigned to them in the PABC-2009. ROMPCS parameter values used in the PCS-

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2012 PA are listed in Table 2-2 and Table 2-3 of Camphouse et al. (2012b). These parameters will also be used in the CRA-2014 PA with a few exceptions. In the PCS-2012 PA, the permeabilities of material PCS_T1 were assigned a uniform distribution having a minimum value of 1 x 10^{-21} m^2. The permeability for material PCS_T2 was calculated as a function of its sampled porosity value. The lowest obtainable calculated value for the permeability of PCS_T2 in the X, Y, and Z directions was 1.44 x 10^{-21} m^2, which is slightly greater than the minimum possible sampled value during the first 100 years. In other words, a lower ROMPCS permeability could be obtained during the first 100 years than was feasible for years 100 to 200, depending on the sampled PCS_T1 permeability value. As creep closure reconsolidates the ROMPCS over time, the expectation is that ROMPCS permeability will not increase as time increases. As a result, the permeability distribution of ROMPCS material PCS_T1 will be modified slightly in the CRA-2014 PA to disallow lower permeability values in years 0 to 100 than are feasible in years 100 to 200. The refined distribution assigned to the log-permeabilities of material PCS_T1 in the CRA-2014 PA is shown in Table 2-1.

Table 2-1: PCS_T1 Log-Permeability Distribution for the CRA-2014 PA

Parameter	Units	Description	Distribution Type	Distribution Parameters	Default Value
PCS_T1:PRMX_LOG[1] PCS_T1:PRMY_LOG PCS_T1:PRMZ_LOG	log(m^2)	$\log_{10}$ of Intrinsic Permeability, X, Y, and Z Directions.	Uniform	Max = -12.0 Mean = -16.42 Min = -20.84	-16.42

The minimum value shown in Table 2-1 yields a permeability of 1.45 x 10^{-21} m^2. This change will not substantively alter repository flow field behavior as the DRZ above and below the ROMPCS is the preferential flow path during years 0 to 200. This parameter change is cosmetic in nature, and is being implemented to improve consistency between the modeled ROMPCS temporal evolution and the mechanics of ROM salt reconsolidation. As was done in the PCS-2012 PA, a conditional relationship will be implemented in the CRA-2014 PA to enforce that the permeability of material PCS_T2 is never greater than the permeability of material PCS_T1. Likewise, the permeability of material PCS_T3 will never be greater than the permeability of material PCS_T2.

For similar reasons, the treatment of materials DRZ_1 and DRZ_PCS will be modified slightly in the CRA-2014 PA as compared to the PCS-2012 PA. It is expected that healing of the DRZ region above and below the ROMPCS after 200 years will not yield an increase in permeability when compared to the damaged DRZ. A relationship will be implemented in the CRA-2014 PA to enforce that the permeability of material DRZ_PCS is never greater than the permeability of material DRZ_1.

Finally, the initial brine saturation of the ROMPCS was obtained through sampling of parameter PCS_T1:SAT_IBRN in the PCS-2012 PA. The random sampling of this parameter resulted in

[1] Parameter values are sampled for PCS_T1:PRMX_LOG. PCS_T1:PRMY_LOG and PCS_T1:PRMZ_LOG inherit the sampled value obtained for PCS_T1:PRMX_LOG for each vector.

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initial brine saturations that were less than the sampled PCS residual brine saturation in some vectors. In the CRA-2014 PA, the initial brine saturation of the ROMPCS will be set equal to the sampled residual brine saturation value for material PCS_T1 in each vector. This modification is being done to ensure that the initial brine saturation of the PCS is never lower than the PCS residual brine saturation in a given vector. This modification will have no impact on compliance results found in the PCS-2012 PA as the DRZ above and below the ROMPCS is the preferential flow path during the first 200 years. A consequence of this change is that parameter PCS_T1:SAT_IBRN will not be used in the CRA-2014 PA.

2.1.2 Additional WIPP Excavated Region

Following the recertification of the WIPP in November of 2010 (U.S. EPA 2010), the DOE submitted a planned change notice (PCN) to the EPA that justified additional excavation in the WIPP experimental area (U.S. DOE, 2011b). This added excavation was proposed in order to support salt disposal investigations (SDI) at WIPP. A performance assessment was undertaken to determine the impact of the additional excavation on the long-term performance of the facility. Impacts were determined via a direct comparison to results obtained in the PABC-2009. It was found that total normalized releases remained below regulatory release limits when the additional excavated volume was added to the repository (Camphouse et al. 2011). Moreover, total normalized releases calculated with the additional excavation were indistinguishable from those obtained in the PABC-2009. After reviewing the DOE proposal and written responses to questions related to the effects of increasing the mining area, the EPA found that the mining phase of the SDI activities will not adversely impact WIPP's waste handling activities, air monitoring, disposal operations, or long-term repository performance (U.S. EPA 2011). Therefore, additional excavation in the WIPP experimental area will be included in the CRA-2014 PA.

2.1.3 Refinement to the Probability of Encountering Pressurized Brine

Penetration into a region of pressurized brine during a WIPP drilling intrusion can have significant consequences with respect to releases. WIPP PA parameter GLOBAL:PBRINE (hereafter PBRINE) is used to specify the probability that a drilling intrusion into the excavated region of the repository encounters a region of pressurized brine below the repository. In the current regulatory baseline established by the PABC-2009, a uniform distribution between 0.01 and 0.60 with a mean value of 0.305 is assigned to this parameter. Initial development of this distribution was the result of an analysis of TDEM data (Rechard et al. 1991, Peake 1998). A framework that provides a quantitative argument for refinement of parameter PBRINE has been developed since the PABC-2009 (Kirchner et al. 2012). The refinement of PBRINE results from a re-examination of the TDEM data while also including a greatly expanded set of drilling data for locations adjacent to the WIPP site than were available when the original analysis was performed in 1998. A sub-region exhibiting a high-density cluster of drilling intrusions was used to provide a conservative estimate of the probability of brine pocket intrusion based solely on the drilling data and to estimate a probability of encountering a brine pocket given that a well is drilled into a TDEM-identified region. The resulting distribution for PBRINE is shown in Table 2-2, and will be used in the CRA-2014 PA.

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Table 2-2: GLOBAL:PBRINE Distribution for the CRA-2014 PA

Parameter	Units	Description	Distribution Type	Distribution Parameters	Default Value
GLOBAL:PBRINE	(none)	Probability that a Drilling Intrusion in Excavated Area Encounters Pressurized Brine	Normal	Mean = 0.127 SD = 0.0272	0.127

As shown in Kirchner et al. (2012), the distribution shown in Table 2-2 will result in simulated frequencies of brine intrusions that cover the same range as that produced using the former uniform distribution, but with a greater degree of positive skewness, resulting in a mode that is shifted to the left.

2.1.4 Refinement to the Corrosion Rate of Steel

The interaction of steel in the WIPP with repository brines will result in the formation of H_2 gas due to anoxic corrosion of the metal. The rate of H_2 gas generation will depend on the corrosion rate and the type of corrosion products formed. Wang and Brush (1996) provided estimates of gas-generation parameters for the long-term WIPP performance assessment based on experimental work of Telander and Westerman (1997). Since the analysis of Wang and Brush, a new series of steel and lead corrosion experiments has been conducted under Test Plan TP 06-02, *Iron and Lead Corrosion in WIPP-Relevant Conditions* (Wall and Enos, 2006). The object of these experiments has been to determine steel and lead corrosion rates under WIPP-relevant conditions. Telander and Westerman measured H_2 generation rates directly and from those measurements were able to calculate metal corrosion rates. In contrast, experiments under Test Plan 06-02 directly measure metal corrosion rates. A description of the new experiments and the use of their results to determine an updated steel corrosion rate are presented in Roselle (2013). WIPP PA parameter STEEL:CORRMCO2 represents the anoxic steel corrosion rate for brine-inundated steel in the absence of microbially produced CO_2. Based on the newly obtained experimental corrosion data and its subsequent analysis, Roselle (2013) recommends that both the distribution type and values for parameter STEEL:CORRMCO2 be changed. The revised steel corrosion parameter is shown in Table 2-3, and will be used for the CRA-2014 PA.

Table 2-3: STEEL:CORRMCO2 Distribution for the CRA-2014 PA

Parameter	Units	Description	Distribution Type	Distribution Parameters	Default Value
STEEL: CORRMCO2	m/s	Rate of anoxic steel corrosion under brine-inundated conditions with no CO_2 present	Student-t (n = 64)	Mean = 6.059e-15 S.D. = 4.047e-15 S.E. = 5.059e-16	6.059e-15

Data used to construct the distribution listed in Table 2-3 are listed in Table 13 of Roselle (2013).

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2.1.5 Refinement to the Effective Shear Strength of WIPP Waste

WIPP PA includes scenarios in which human intrusion results in a borehole intersecting the repository. During the intrusion, drilling mud flowing up the borehole will apply a hydrodynamic shear stress on the borehole wall. Erosion of the wall material can occur if this stress is high enough, resulting in a release of radionuclides being carried up the borehole with the drilling mud. In this intrusion event, the drill bit would penetrate repository waste, and the drilling mud would flow up the borehole in a predominately vertical direction. In order to experimentally simulate these conditions, a flume was designed and constructed. In the flume experimental apparatus, eroding fluid enters a vertical channel from the bottom and flows past a specimen of surrogate WIPP waste. Experiments were conducted to determine the erosive impact on surrogate waste materials that were developed to represent WIPP waste that is 50%, 75%, and 100% degraded by weight. A description of the vertical flume, the experiments conducted in it, and conclusions to be drawn from those experiments are discussed in Herrick et al. (2012). WIPP PA parameter BOREHOLE:TAUFAIL is used to represent the effective shear strength for erosion of WIPP waste. Based on experimental results that realistically simulate the effect of a drilling intrusion on an accepted surrogate waste material, as well as analyses of existing data, Herrick (2013) recommends a refinement to parameter BOREHOLE:TAUFAIL. The refinement of this parameter is shown in Table 2-4, and will be used in the CRA-2014 PA.

Table 2-4: BOREHOLE:TAUFAIL Distribution for the CRA-2014 PA

Parameter	Units	Description	Distribution Type	Distribution Parameters	Default Value
BOREHOLE: TAUFAIL	Pa	Effective shear strength for erosion of waste.	Uniform	Max = 77.0 Mean = 39.61 Min = 2.22	39.61

2.1.6 Updates to Drilling Rate and Plugging Pattern Parameters

WIPP regulations require that current drilling practices are 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. Results for the year 2012 are documented in the 2012 Delaware Basin Monitoring Annual Report (U.S. DOE/WIPP 2012). The 2012 summary report shows that drilling practices have not changed since the summary report used for the PABC-2009.

Drilling parameters will be updated for the CRA-2014 PA to include information assembled through 2012. The 2012 Delaware Basin Monitoring Annual Report (U.S. DOE/WIPP 2012) indicates a drilling rate of 67.3 boreholes per km^2 over 10,000 years, resulting in a value for WIPP PA parameter GLOBAL:LAMBDAD of 6.73×10^{-3} boreholes per km^2 per year in the CRA-2014 PA. This is an increase to the value of 5.98×10^{-3} specified for this parameter in the PABC-2009. The percentage of boreholes that are plugged all through the salt section (WIPP PA parameter GLOBAL:ONEPLG, shown as type VI in Table 10 of U.S. DOE/WIPP 2012) is 4.0%, an increase of 1.8% to the value prescribed to this parameter in the PABC-2009. The

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percentage of boreholes with a plug between the repository and a hypothetical brine pocket (WIPP PA parameter GLOBAL:THREEPLG, shown as types II and IV in Table 10 of U.S. DOE/WIPP 2012) is 36.6%, an increase when compared to the value of 32.6% used for this parameter in the PABC-2009. The remaining plugging pattern (WIPP PA parameter GLOBAL:TWOPLG, shown as types I, III, and V in Table 10 of U.S. DOE/WIPP 2012) is 59.4%, a reduction to the value of 65.2% used in the PABC-2009. These parameters are summarized in Table 2-5.

Table 2-5: Drilling Rate and Plugging Pattern Parameters for the CRA-2014 PA

Parameter	Units	Description	Distribution Type	Value
GLOBAL: LAMBDAD	km^{-2} yr^{-1}	Drilling rate per unit area	Constant	6.73×10^{-3}
GLOBAL: ONEPLG	(none)	Probability of having Plug Pattern 1	Constant	0.04
GLOBAL: TWOPLG	(none)	Probability of having Plug Pattern 2	Constant	0.594
GLOBAL: THREEPLG	(none)	Probability of having Plug Pattern 3	Constant	0.366

2.1.7 Updates to WIPP Waste Inventory Parameters

The Performance Assessment Inventory Report (PAIR) – 2012 (Van Soest 2012) was released on November 29, 2012. The PAIR – 2012 contains updated estimates to the radionuclide content and waste material parameters, scaled to a full repository, based on inventory information collected up to December 31, 2011. In order to incorporate this update to the inventory into the CRA-2014 PA, the parameters for the initial radionuclides, chemical components and waste material inventories will be updated. In addition, parameters which are calculated based on the initial radionuclide inventories, such as the Waste Unit Factor (WUF) and the initial lumped radionuclide inventories will be updated as well. Inventory parameters to be updated in the CRA-2014 PA are listed in Table 2-6. Along with the parameter updates shown in Table 2-6, the analysis of the radionuclides that dominate releases will be updated.

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Table 2-6: Inventory Parameters for the CRA-2014 PA

Materials	Properties	Description
AM241, AM243, CF252, CM243, CM244, CM245, CM248, CS137, NP237, PA231, PB210, PM147, PU238, PU238, PU240, PU241, PU242, PU244, RA226, RA228, SR90, TH229, TH230, TH232, U233, U234, U235, U236, U238	INVCHD and INVRHD	WIPP-Scale Initial Radionuclide Inventory in Curies
AM241L, TH230L, PU238L, U234L, PU239L	INVCHD and INVRHD	WIPP-Scale Initial Lumped Radionuclide Inventory in Curies
BOREHOLE	WUF	Waste Unit Factor
NITRATE, SULFATE	QINIT	WIPP-Scale Amounts of Nitrate and Sulfate (in moles)

Masses of waste and packaging materials are given in the PAIR – 2012, whereas the densities of these materials were reported in prior inventory reports. The reporting of mass for these materials allows for more transparent treatment of them in PA. Previously, reported densities were converted to mass values during pre-processing. The reporting of mass allows for reported quantities to be directly used in PA. The change from density to mass requires new waste area parameters that represent mass values reported in the PAIR – 2012. These new parameters are shown in Table 2-7.

Table 2-7: Waste Area Inventory Parameters for the CRA-2014 PA

Materials	Properties	Description
WAS_AREA	IRONCHW, IRONRHW, IRNCCHW, IRNCRHW, CELLCHW, CELLRHW, CELCCHW, CELCRHW, CELECHW, CELERHW, PLASCHW, PLASRHW, PLSCCHW, PLSCRHW, PLSECHW, PLSERHW, RUBBCHW, RUBBRHW, RUBCCHW, RUBCRHW, RUBECHW, RUBERHW	Waste Material Parameters

The PAIR - 2012 also includes information on the volume and radionuclide content for each waste stream. This information is used to generate the probability of encountering a waste stream and the normalized release as a function of time for each waste stream. Waste stream

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information is stored in the input files for WIPP PA code EPAUNI. These input files will be updated in the CRA-2014 PA to reflect the most current waste stream information.

2.1.8 Implementation of Variable Brine Volume in the Calculation of Radionuclide Concentration

In the PABC-2009, the minimum necessary brine volume in the repository for a direct brine release (DBR) to occur was established as 17,400 m^3 (Clayton 2008). This value will also be used in the CRA-2014 PA as no changes warranting an update to it have occurred since the PABC-2009. The minimum brine volume necessary for a DBR is used in the calculation of radionuclide brine concentrations. The increasing WIPP organic ligand inventory has resulted in mass-balance issues when determining radionuclide concentrations from only the minimum brine volume necessary for a DBR. As a result, the calculation of radionuclide concentrations in brine will be extended in the CRA-2014 PA so that concentrations are dependent on the actual volume of brine present in the repository. This will result in radionuclide concentrations in brine that are more defensible.

To date, the minimum brine volume necessary for a DBR has been used as an input to the radionuclide solubility calculation. The entire organic ligand inventory was assumed to be dissolved in the minimum necessary DBR brine volume, and the resulting organic ligand concentrations were then used in the calculation of radionuclide solubilities. As the organic ligand inventory has increased over time, the use of a constant organic ligand concentration in brine that is independent of the actual volume of brine present in the repository has resulted in overall mass-balance errors when repository brine volumes are larger than the minimum necessary for a DBR. Using results from previous DBR calculations, DBR volumes realized in PA are between the necessary minimum volume and five times the minimum brine volume. As a result, brine volumes of 1x, 2x, 3x, 4x, and 5x the minimum necessary volume will be used in the calculation of radionuclide concentration. The organic ligand inventory will be dissolved in each of these multiples of the minimum necessary brine volume. The resulting organic ligand concentrations, now dependent on a range of brine volume, will be used to calculate radionuclide solubilities. This approach will keep radionuclide mass constant over realized brine volumes, rather than keeping radionuclide concentration constant over realized brine volumes. The use of five multiples of the minimum necessary DBR volume provides a sufficient range with which to calculate solubilities while keeping the additional solubility calculation workload at a feasible level.

Radionuclide concentrations prescribed for a particular DBR volume will be obtained by interpolating between concentrations calculated for the integer multiples of the minimum necessary DBR volume. This will yield a radionuclide concentration consistent with the actual brine volume present in the repository. WIPP PA codes PRECCDFGF v2.0 and CCDFGF v6.0 have been developed and qualified for this revised implementation of radionuclide concentration as a function of brine volume.

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2.1.9 Updates to Radionuclide Solubilities

The solubilities of actinide elements are influenced by the chemical components of the waste. With the release of the PAIR - 2012 (Van Soest 2012), updated information on the amount of various chemical components in the waste is available. To incorporate this updated information, parameters used to represent actinide solubilities will be updated in the CRA-2014 PA. Additional experimental results have been published in the literature since the PABC-2009, and this new information will be used to enhance the uncertainty ranges and probability distributions for actinide solubilities. Details of the development of radionuclide solubilities and their associated uncertainty for the CRA-2014 PA are contained in *Analysis Plan for WIPP Near-Field Geochemical Process Modeling, AP-153* (Brush et al. 2012). Table 2-8 lists solubility parameters that will be used in the CRA-2014 PA. Parameters in roman font in Table 2-8 are established parameters that will have their values updated from those used in the PABC-2009. Parameters with italicized font are new parameters that will be created in the CRA-2014 PA. These new parameters will represent solubilities that are calculated using multiples of the minimum brine volume necessary for a DBR to occur. For these parameters, the numerical suffix indicates the minimum brine volume multiple used to calculate the solubility. For example, *SOLCOH2* is calculated using 2x the minimum necessary brine volume, *SOLCOH3* is calculated using 3x the minimum necessary brine volume, etc.

Table 2-8: Solubility Parameters for the CRA-2014 PA

Materials	Properties	Description
SOLMOD3, SOLMOD4	SOLCOH, SOLSOH, SOLVAR *SOLCOH2, SOLSOH2,* *SOLCOH3, SOLSOH3,* *SOLCOH4, SOLSOH4,* *SOLCOH5, SOLSOH5*	Actinide Solubilities in Castile and Salado Brines
SOLMOD5	SOLCOH, SOLSOH *SOLCOH2, SOLSOH2,* *SOLCOH3, SOLSOH3,* *SOLCOH4, SOLSOH4,* *SOLCOH5, SOLSOH5*	

2.1.10 Refinement to Repository Water Balance[2]

The saturation and pressure history of the repository are used throughout PA. Along with flow in and out of the repository, the saturation and pressure are influenced by the reaction of materials placed in the repository with the surrounding environment. In the implementation used for the PABC-2009, the anoxic corrosion reaction of iron to form iron hydroxide,

$$Fe(s) + 2\ H_2O(g,l) \rightarrow H_2(g) + Fe(OH)_2(s),$$

[2] The author wishes to acknowledge the contribution of Daniel Clayton, SNL Org 6223, in the preparation of Section 2.1.10.

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is included as a brine-consuming and gas-producing reaction in the repository. Additionally, the biodegradation of cellulose, plastic and rubber (CPR), which assumes microbial consumption of cellulose, $C_6H_{10}O_5$,

$$C_6H_{10}O_5(s) + \text{microbes} \rightarrow H_2(g) + \text{unknowns},$$

is incorporated as a source of gas. Furthermore, the iron sulfidation and MgO carbonation reactions,

$$Fe(s) + H_2S(g) \rightarrow FeS(s) + H_2(g), \text{ and}$$

$$MgO(s) + CO_2(g,aq) \rightarrow MgCO_3(s),$$

are implicitly included.

As part of the review of the CRA-2009, EPA noted several issues for possible additional investigation, including the potential implementation of a more detailed repository water balance (U.S. EPA 2010b). The main objective of refining the repository water balance is to include the major gas and brine producing and consuming reactions in the existing conceptual model. As described in the Chemical Conditions Conceptual Model, the major reactions in the repository include CPR, iron and MgO (U.S. DOE 2004, sections PEER-2004 1.1.3, PEER-2004 1.1.4 and PEER-2004 1.1.5).

The major pathways for biodegradation include the following reactions:

$$C_6H_{10}O_5(s) + 4.8\ H^+(aq) + 4.8\ NO_3^-(aq) \rightarrow 7.4\ H_2O(l) + 6\ CO_2(g) + 2.4\ N_2(g)$$

$$C_6H_{10}O_5(s) + 6\ H^+(aq) + 3\ SO_4^{2-}(aq) \rightarrow 5\ H_2O(l) + 6\ CO_2(g) + 3\ H_2S(g)$$

$$C_6H_{10}O_5(s) + H_2O(g,l) \rightarrow 3\ CH_4(g) + 3\ CO_2(g)$$

These reactions are assumed to proceed sequentially, consuming the limited amount of nitrate (NO_3^-) and sulfate (SO_4^{2-}) in the repository. Currently, it is assumed that there is sufficient sulfate in the surrounding rock to consume all the CPR and hence the last reaction is not used. Furthermore, in the PABC-2009 it was assumed that the biodegradation reactions neither consume nor produce water. For the CRA-2014, the same biodegradation pathways will be included as implemented in the PABC-2009, but the generation of water will also be considered.

In the CRA-2014, in addition to the iron corrosion and sulfidation reactions discussed above, the reaction of iron hydroxide with hydrogen sulfide,

$$Fe(OH)_2(s) + H_2S(g) \rightarrow FeS(s) + 2\ H_2O(l),$$

which consumes gas and produces water, will also be included.

For the CRA-2014, the MgO reactions will be expanded to include MgO hydration,

$$MgO(s) + H_2O(g,l) \rightarrow Mg(OH)_2(s),$$

which consumes water and produces brucite [$Mg(OH)_2$], and the carbonation of brucite to form hydromagnesite [$Mg_5(CO_3)_4(OH)_2{:}4H_2O$],

$$5\ Mg(OH)_2(s) + 4\ CO_2(g,aq) \rightarrow Mg_5(CO_3)_4(OH)_2{:}4H_2O(s).$$

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Since hydromagnesite is not thermodynamically stable under repository conditions, it is expected to dehydrate to form magnesite. For the CRA-2014, the reaction of hydromagnesite to form magnesite ($MgCO_3$),

$$Mg_5(CO_3)_4(OH)_2{:}4\ H_2O(s) \rightarrow 4\ MgCO_3(s) + Mg(OH)_2(s) + 4\ H_2O(l),$$

which produces water, will also be included.

To include these additional reactions, the stoichiometric coefficient matrix values will be updated and parameters will be added that represent hydromagnesite (density and molecular weight) and the rate of the hydromagnesite conversion to magnesite. Additionally, since the parameters for the MgO hydration were implemented, updated information on the reaction rate has been generated, and so these values will be updated. All the parameters that will be changed or created to include this refinement to the repository water balance are shown in Table 2-9. WIPP PA codes PREBRAG v8.02 and BRAGFLO v6.02 have been developed and qualified for this refinement to the repository water balance.

Table 2-9: Additional Chemistry Parameters for the CRA-2014 PA

Material	Properties	Description
REFCON	DN_HYDRO	Hydromagnesite Density
REFCON	MW_HYDRO	Hydromagnesite Molecular Weight
REFCON	STCO_*xy*	Stoichiometric Coefficients for Reaction *x*, Species *y*
WAS_AREA	BRUCITEC, BRUCITES	MgO Inundatated Hydration Rate in Castile and Salado Brines
WAS_AREA	BRUCITEH	Humid MgO hydration rate
WAS_AREA	HYMAGCON	Hydromagnesite Conversion Rate

2.1.11 Parameter Corrections

PA material DRZ_PCS was developed in 2002 to represent healed portions of the DRZ above a panel closure (Stein 2002). As developed in 2002, it was intended that property values assigned to material DRZ_PCS be exactly the same as those used for material DRZ_1, with the exception of log-permeabilities in the X, Y, and Z directions. Parameter DRZ_1:RELP_MOD is assigned a Delta distribution having a minimum of 1, a maximum of 4, with the mean, median, and default value all assigned a value of 4. The (probability,value) pairs assigned to parameter DRZ_1:RELP_MOD are (0.33,1), (0,2), (0,3), and (0.67,4). Conversely, the Delta distribution entered into the PA parameter database for parameter DRZ_PCS:RELP_MOD has a minimum of 1, a maximum of 4, the same probability pairs as DRZ_1:RELP_MOD, but a mean, median, and default value of 0. To bring parameter DRZ_PCS:RELP_MOD into agreement with the justification used in its original 2002 development, it will be updated in the CRA-2014 PA so that it is identical to parameter DRZ_1:RELP_MOD. The revised distribution for parameter DRZ_PCS:RELP_MOD is shown in Table 2-10.

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Table 2-10: DRZ_PCS:RELP_MOD Distribution for the CRA-2014 PA

Parameter	Units	Description	Distribution Type	Distribution Values	Default Value
DRZ_PCS: RELP_MOD	(none)	Model number, relative permeability number	Delta	Max = 4 Mean = 4 Median = 4 Min = 1 SD = 0 (Prob., Value) Pairs: (0.33,1) (0,2) (0,3) (0.67,4)	4

Note that this refinement to parameter DRZ_PCS:RELP_MOD will have no impact on computed PA results. Values of DRZ_PCS:RELP_MOD are inherited from those obtained for DRZ_1:RELP_MOD in the Algebra1 input file to BRAGFLO, and have been since the TBM PA. The refinement of parameter DRZ_PCS:RELP_MOD is cosmetic is nature, and is being done to enhance agreement between the historical development of this parameter and the values entered into the PA parameter database.

2.2 *FEPs Re-assessment*

An assessment of the FEPs baseline will be conducted to determine if the FEPs basis remains valid in consideration of changes introduced by the CRA-2014 PA. Results of this FEPs assessment will be documented in a separate report.

2.3 *Calculation Methodology*

2.3.1 Rationale

The aim of the CRA-2014 PA is to quantify regulatory compliance impacts associated with changes made since the PABC-2009. Impacts will be determined by a direct comparison of CRA-2014 PA and PABC-2009 results. As seen in Section 2.1, changes incorporated into the CRA-2014 PA include planned changes as well as parameter and implementation changes. The approach taken in the CRA-2014 PA is to reasonably isolate impacts associated with these changes, and then to assess the combined impact when all are included in the PA. To that end, a number of individual cases will be investigated in the CRA-2014 PA. These cases are now discussed.

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2.3.1.1 Case CRA14-BL

The first case considered in the CRA-2014 PA will be used to compare the impact of a baseline set of changes relative to the PABC-2009. The name given to this case is CRA14-BL (for CRA-2014 Baseline). Regulatory compliance impacts associated with replacement of the Option D panel closure with the ROMPCS design are discussed and compared to PABC-2009 results in Camphouse et al. (2012b). Similarly, impacts of additional mining in the WIPP experimental area are assessed via a comparison to PABC-2009 results in Camphouse et al. (2011). Consequently, these two planned changes will be included in case CRA14-BL as their impacts have already been assessed via comparisons to the PABC-2009. In addition to these two planned changes, "standard" updates typically included in a re-certification PA will also be included in the baseline case. These standard updates consist of changes to repository inventory information obtained since the most recent re-certification (see Table 2-6 and Table 2-7), updates to radionuclide solubilities to account for the new inventory information (see Table 2-8), and updates to repository drilling rates and plugging patterns (see Table 2-5). Case CRA14-BL will utilize this baseline set of changes and assess their impact in relation to PABC-2009 results. Case CRA14-BL will not include an updated distribution for iron corrosion, a refined water balance that includes MgO hydration, the implementation of variable brine volumes in the calculation of DBRs, or updated distributions for parameters GLOBAL:PBRINE and BOREHOLE:TAUFAIL. Changes considered in Case CRA14-BL will be limited to

- Replacement of Option D with the ROMPCS
- Additional excavation in the WIPP experimental area
- Updated waste inventory parameters
- Updated radionuclide solubilities and their associated uncertainty, with solubilities calculated using only the minimum necessary brine volume for a DBR
- Updated drilling rate and plugging pattern parameters

A single replicate (Replicate 1) will be executed for Case CRA14-BL and used to ascertain regulatory compliance impacts associated with the set of baseline changes in the CRA-2014 PA. Impacts will be assessed via a direct comparison of Case CRA14-BL Replicate 1 results to PABC-2009 Replicate 1 results.

2.3.1.2 Case CRA14-TP

With the results of case CRA14-BL in hand, two parameter updates will be added to the set of baseline changes so that their impacts can be determined. The addition of these changes, and their impact on regulatory compliance, will be captured in case CRA14-TP (for CRA-2014 (T)AUFAUL (P)BRINE). Refinements to the waste shear strength and the probability of encountering a pressurized brine pocket during a drilling intrusion have distinct impacts on WIPP release pathways. The updated distribution for parameter BOREHOLE:TAUFAIL will potentially alter cavings releases in comparison to PABC-2009 results. Updating parameter GLOBAL:PBRINE will primarily impact DBRs with secondary impacts possible for long-term transport releases. As these two parameter changes lead to distinct impacts, case CRA14-TP will consist of a focused re-run of case CRA14-BL with updated distributions implemented for

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parameters BOREHOLE:TAUFAIL and GLOBAL:PBRINE. As described for case CRA14-BL, case CRA14-TP will consist of a single replicate (Replicate 1). Results obtained from case CRA14-TP will be compared to Replicate 1 results obtained in the PABC-2009, with discussion of CRA14-BL results where appropriate.

In summary, case CRA14-TP will incorporate changes included in case CRA14-BL as well as refinements to parameters BOREHOLE:TAUFAIL and GLOBAL:PBRINE.

2.3.1.3 Case CRA14-BV

The focus of case CRA14-BV (for CRA-2014 (B)rine (V)olumes) is to assess the impact of the variable brine volume implementation on results calculated in case CRA14-TP. Thus, case CRA14-BV will consist of a focused re-run of case CRA14-TP, and will incorporate radionuclide concentrations based on 1x, 2x, 3x, 4x, and 5x the minimum requisite brine volume for a DBR. As before, a single replicate (Replicate 1) will be executed for CRA14-BV, with results compared to Replicate 1 results of the PABC-2009. Case CRA14-BV results will also be compared with CRA14-TP results as appropriate. Case CRA14-BV will incorporate all changes included in case CRA14-TP as well as the implementation of variable brine volume in the calculation of radionuclide concentrations in brine.

2.3.1.4 Case CRA14-0

Case CRA14-0 will incorporate all changes included in the CRA-2014 PA. That is, case CRA14-0 will include all changes described for case CRA14-BV as well as the refinements to the steel corrosion rate (see Table 2-3) and a water balance that includes MgO hydration (see Section 2.1.10). Three replicates will be executed for case CRA14-0, with results being compared to those obtained in the PABC-2009. Case CRA14-0 results for Replicate 1 will also be compared to CRA12-BV results as appropriate.

2.3.1.5 Summary of CRA-2014 PA Cases

A summary of the cases discussed in Section 2.3.1 is shown in Table 2-11.

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Table 2-11: Cases Considered in the CRA-2014 PA

	CRA-2014 PA Cases			
	Case CRA14-BL	Case CRA14-TP	Case CRA14-BV	Case CRA14-0
CRA-2014 PA changes included	Replacement of Option D PCS with the ROMPCS Inclusion of additional mined region in the WIPP experimental area Updated WIPP waste inventory parameters Updated radionuclide solubilities and uncertainty Updated drilling rate and plugging pattern parameters	Replacement of Option D PCS with the ROMPCS Inclusion of additional mined region in the WIPP experimental area Updated WIPP waste inventory parameters Updated radionuclide solubilities and uncertainty Updated drilling rate and plugging pattern parameters BOREHOLE:TAUFAIL and GLOBAL:PBRINE parameter distribution refinements	Replacement of Option D PCS with the ROMPCS Inclusion of additional mined region in the WIPP experimental area Updated WIPP waste inventory parameters Updated radionuclide solubilities and uncertainty Updated drilling rate and plugging pattern parameters BOREHOLE:TAUFAIL and GLOBAL:PBRINE parameter distribution refinements Variable Brine Volume Implementation	Replacement of Option D PCS with the ROMPCS Inclusion of additional mined region in the WIPP experimental area Updated WIPP waste inventory parameters Updated radionuclide solubilities and uncertainty Updated drilling rate and plugging pattern parameters BOREHOLE:TAUFAIL and GLOBAL:PBRINE parameter distribution refinements Variable Brine Volume Implementation Update to parameter STEEL:CORRMCO2 Refinement to Repository Water Balance Implementation
Number of replicates	1	1	1	3

2.3.2 Code Execution

As described above, planned changes, parameter changes, and implementation refinements will be incorporated into the CRA-2014 PA in a sequential fashion so that their impacts can be reasonably isolated. This sequential inclusion of change results in code executions that are different for the four cases described in Section 2.3.1. The sequence of code execution used in the CRA-2014 PA for each of the four cases is now described.

2.3.2.1 Code Execution for Case CRA14-BL

Changes incorporated into case CRA14-BL include two planned changes that impact repository pressure and brine saturation as compared to PABC-2009 results, updates to waste inventory parameters as well as updates to individual waste streams represented in the CRA-2014 PA, updated radionuclide solubilities which potentially impact the concentration of waste in brine, and updated drilling rate and plugging pattern parameters that impact the frequency of drilling intrusion. Case CRA14-BL will consist of a single replicate (Replicate 1) consisting of 100 vectors. The structure of the calculations that will be performed for case CRA14-BL is listed below.

Parameter Sampling: LHS

One replicate of 100 vectors will be created using the computer code LHS. LHS sampling in case CRA14-BL will be done to reflect sampled CRA-2014 PA parameters listed under case CRA14-BL in Table 2-11. Parameter distributions used in the PABC-2009 will be used for sampled parameters not listed under case CRA14-BL in Table 2-11. LHS version 2.42 will be used for the CRA-2014 PA, which is the same code used for the PABC-2009. The random seed and parameter ordering from Replicate 1 of the PABC-2009 will be used for case CRA14-BL in the CRA-2014 PA. Use of the PABC-2009 random seeds and ordering will result in identical sampled values for sampled parameters that are common to both case CRA14-BL and Replicate 1 of the PABC-2009. This approach enables comparison of case CRA14-BL and PABC-2009 results on a vector-by-vector basis.

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-BF to S5-BF are used as input for the subsequent calculation of Salado radionuclide transport, DBRs, and spallings releases. BRAGFLO scenario S6-BF is used in the calculation of radionuclide transport to the Culebra. The scenarios modeled in BRAGFLO are listed in Table 2-12.

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Table 2-12: WIPP PA BRAGFLO Scenarios

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

Implementation of the ROMPCS and the additional excavated region in the WIPP experimental area will slightly alter the BRAGFLO computational grid and material maps as compared to those used in the PABC-2009. Discussions of these changes can be found in Camphouse et al. (2012b) and Camphouse et al. (2011).

A single BRAGFLO replicate (Replicate 1) will be executed for case CRA-2014-BL. The calculation will consist of 100 vectors over 6 scenarios (see Table 2-12). The codes PREBRAG version 8.0, BRAGFLO version 6.0, and POSTBRAG version 4.00A will be used for case CRA14-BL, and are the same code versions used in the PABC-2009.

Direct Solids Releases: DRSPALL and CUTTINGS_S

Updated waste inventory information included in the CRA-2014 PA can potentially change cuttings and cavings releases as compared to the PABC-2009. Repository pressures will be affected by the implementation of the ROMPCS design and inclusion of additional excavation in the WIPP experimental area. Changes in repository pressures have the potential to impact spallings results. Consequently, direct solids releases for the CRA-2014 PA may differ from those found in the PABC-2009 due to differences in repository pressures calculated by BRAGFLO as well as updated inventory information. Spallings volumes from a single borehole intrusion are calculated by code DRSPALL at initial repository pressures of 10, 12, 14, and 14.8 MPa. DRSPALL calculations that were utilized to generate spallings volumes at these pressures in the PABC-2009 will also be used in the CRA-2014 PA. The CRA-2014 PA will use the same procedure as was used for the PABC-2009 to interpolate between these DRSPALL volumes to calculate spallings volumes corresponding to a particular drilling intrusion. The initial repository pressure for a given scenario, time, location, and vector will be retrieved from the BRAGFLO results, and CUTTINGS_S will use this initial pressure to calculate a spallings volume for each scenario, time, location, and vector combination by interpolating between DRSPALL results. The code CUTTINGS_S version 6.02 will be used for the CRA-2014 PA, which is the same code used for the PABC-2009. Direct solids releases will be calculated for one replicate (Replicate 1) in case CRA14-BL.

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Actinide Mobilization: PANEL

WIPP PA code PANEL calculates quantities of actinides mobilized by colloids and as dissolved species in WIPP brines. PANEL uses actinide solubilities from the WIPP parameter database, and these parameters will be updated for the CRA-2014 PA (see Table 2-8). As a result, PANEL will be executed for one replicate (Replicate 1) in case CRA14-BL. In case CRA14-BL, PANEL will only use solubilities calculated with the minimum necessary brine volume for a DBR. PANEL version 4.03 will be used for the CRA-2014 PA, which is the same code utilized to generate the actinide mobilization used for the PABC-2009.

Salado Transport: NUTS and PANEL

Changes incorporated into case CRA14-BL potentially impact waste concentrations in brine as well as repository conditions found with BRAGFLO. The WIPP radioisotope mobilization and decay code NUTS is used to simulate the transport of radionuclides through the Salado Formation for scenarios S1-BF through S5-BF. A single replicate (Replicate 1) of NUTS calculations will be executed for case CRA14-BL. NUTS version 2.05C will be used for the CRA-2014 PA, which is the same code used for the PABC-2009.

Based on drilling event characteristics, intrusions are classified as no change (not significantly changing repository behavior), an E1 type (where a region of pressurized brine is encountered) or an E2 type (where pressurized brine pocket is not encountered). Radionuclide transport to the Culebra for the E2E1 intrusion combination (BRAGFLO scenario S6-BF) is calculated by running the PANEL code in "intrusion mode" (PANEL_INT). A single replicate (Replicate 1) of PANEL_INT calculations will be performed for case CRA14-BL using the same procedure that was used in the PABC-2009 PANEL_INT calculations. The code PANEL version 4.03 will be used for the CRA-2014 PA, which is the same code version used for the PABC-2009.

Direct Brine Releases: BRAGFLO

In addition to its role as a tool used to simulate brine and gas flow in and around the WIPP repository, BRAGFLO is also used in PA to calculate DBR volumes. As the changes incorporated in case CRA14-BL will potentially impact pressure and brine saturation in waste-containing repository regions, DBR calculations consisting of a single replicate (Replicate 1) will be performed as part of case CRA14-BL. The numerical grid and material map used to calculate DBRs will be updated to reflect the ROMPCS design as discussed in Malama (2012). Conditions required for the initiation of a DBR release will remain unchanged from the PABC-2009, and the DBR volumes will be calculated for the same scenarios and times (see Table 2-13). The codes PREBRAG version 8.0, BRAGFLO version 6.0, and POSTBRAG version 4.00A will be used for case CRA14-BL, and are the same code versions used in the PABC-2009.

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Table 2-13: PA Intrusion Scenarios Used in Calculating Direct Brine Releases

Scenario	Conditioning (or 1st) Intrusion Time (year) and Type	Intrusion Times – Subsequent (year)
S1-DBR	None	100, 350, 1000, 3000, 5000, 10000
S2-DBR	350, E1	550, 750, 2000, 4000, 10000
S3-DBR	1000, E1	1200, 1400, 3000, 5000, 10000
S4-DBR	350, E2	550, 750, 2000, 4000, 10000
S5-DBR	1000, E2	1200, 1400, 3000, 5000, 10000

Culebra Flow and Transport: MODFLOW and SECOTP2D

Culebra flow and transport calculations will be identical to those found in the PABC-2009 because their parameters and conceptual models are not impacted by any of the updates or corrections implemented in the CRA-2014 PA. Consequently, the Culebra flow and transport results from the PABC-2009 will be used for the CRA-2014 PA. These results are documented in Kuhlman (2010).

CCDF Construction: CCDFGF

The CRA-2014 PA will calculate CCDFs of individual vectors for total normalized releases, cuttings and cavings releases, spallings releases, DBRs, and releases from the Culebra. Mean CCDFs for each release pathway will be calculated for Replicate 1 in case CRA14-BL. The 95% confidence limit on the mean will also be calculated. The codes EPAUNI version 1.15A, PRECCDFGF version 2.0 and CCDFGF version 6.0 will be used for the CRA-2014 PA. EPAUNI input files will be updated in the CRA-2014 PA to include new waste stream information contained in the PAIR – 2012 (Van Soest 2012). PRECCDFGF v2.0 and CCDFGF v6.0 have been developed and qualified since the PABC-2009 to incorporate the implementation of radionuclide concentration as a function of brine volume. CCDFGF calculations in case CRA14-BL will only utilize PANEL actinide mobilization results corresponding to the minimum repository brine volume necessary for a DBR.

2.3.2.2 Code Execution for Case CRA14-TP

As discussed in Section 2.3.1.2 and summarized in Table 2-11, case CRA14-TP is an extension of case CRA14-BL that includes refinements to distributions prescribed to parameters BOREHOLE:TAUFAIL and GLOBAL:PBRINE. Changes to these parameters do not impact the entire code execution chain used for case CRA14-BL. In fact, results obtained in case CRA14-BL will also be used in case CRA14-TB with a few exceptions. These exceptions are now discussed.

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Parameter Sampling: LHS

Parameter values prescribed to BOREHOLE:TAUFAIL and GLOBAL:PBRINE in a given vector are sampled. As a result, parameter sampling performed in case CRA14-BL will be modified in case CRA14-TP to also include sampling of the refined distributions assigned to parameters BOREHOLE:TAUFAIL and GLOBAL:PBRINE. One replicate of 100 vectors will be created using the computer code LHS. LHS sampling in case CRA14-TP will be done to reflect sampled CRA-2014 PA parameters listed under case CRA14-TP in Table 2-11. Parameter distributions used in the PABC-2009 will be used for sampled parameters not listed under case CRA14-TP in Table 2-11. The random seed and parameter ordering from Replicate 1 of the PABC-2009 will be used for case CRA14-TP in the CRA-2014 PA.

Cavings Releases: CUTTINGS_S

Refinement to the waste shear strength will impact cavings release volumes calculated by code CUTTINGS_S. As a result, code CUTTINGS_S will be re-run in case CRA14-TP, and will use the updated BOREHOLE:TAUFAIL sampled values generated by code LHS. Updated cuttings and cavings release volumes will be calculated for one replicate (Replicate 1) in case CRA14-TP.

CCDF Construction: CCDFGF

Parameter GLOBAL:PBRINE is used by code CCDFGF to determine the probability of encountering a region of pressurized brine during a drilling intrusion. As a result, refinement to this parameter potentially impacts results obtained with CCDFGF. Likewise, refinement to parameter BOREHOLE:TAUFAIL will impact release volumes that are used by code CCDFGF to construct direct solids releases. Consequently, code CCDFGF will be re-run in case CRA14-TP to capture release impacts associated with updates to parameters GLOBAL:PBRINE and BOREHOLE:TAUFAIL. Mean CCDFs for each release pathway will be calculated for Replicate 1 in case CRA14-TP. The 95% confidence limit on the mean will also be calculated. CCDFGF calculations in case CRA14-TP will utilize PANEL actinide mobilization results generated in case CRA14-BL that correspond to the minimum repository brine volume necessary for a DBR.

2.3.2.3 Code Execution for Case CRA14-BV

As discussed in Section 2.3.1.3 and summarized in Table 2-11, case CRA14-BV is a modification to case CRA14-TP that includes the implementation of variable brine volume in the calculation of radionuclide concentrations in brine. The implementation of variable brine volume does not impact the entire code execution chain used for case CRA14-TP. Results obtained in case CRA14-TP will also be used in case CRA14-BV with a few exceptions. These exceptions are now discussed.

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Actinide Mobilization: PANEL

As seen in Table 2-8, radionuclide solubilities will be calculated in the CRA-2014 PA in terms of 1x, 2x, 3x, 4x, and 5x the minimum repository brine volume necessary for a DBR. As code PANEL uses actinide solubilities from the WIPP database, and these solubilities will be calculated over multiple brine volumes in the CRA-2014 PA, PANEL input files used in case CRA14-BL will be modified in case CRA14-BV to include these additional solubility parameters. With the modified input files in hand, PANEL will be executed for one replicate (Replicate 1) in case CRA14-BV, yielding results that incorporate the full set of solubilities listed in Table 2-8.

CCDF Construction: CCDFGF

The implementation of variable brine volume in the calculation of radionuclide brine concentration will impact CCDFGF results corresponding to DBR releases. Consequently, code CCDFGF will be re-run in case CRA14-BV to capture release impacts associated with the implementation of variable brine volume. Mean CCDFs for each release pathway will be calculated for Replicate 1 in case CRA14-BV. The 95% confidence limit on the mean will also be calculated. CCDFGF calculations in case CRA14-BV will utilize PANEL actinide mobilization results generated in case CRA14-BV that correspond to 1x, 2x, 3x, 4x, and 5x the minimum repository brine volume necessary for a DBR.

2.3.2.4 Code Execution for Case CRA14-0

As discussed in Section 2.3.1.4 and summarized in Table 2-11, case CRA14-0 is a modification to case CRA14-BV that includes an update to parameter STEEL:CORRMCO2 and a refinement to the repository water balance implementation. As such, case CRA14-0 incorporates all of the changes included in the CRA-2014 PA. Case CRA14-0 will consist of a full set of PA compliance calculations. That is, three replicates, with each replicate consisting of 100 vectors, will be produced for case CRA14-0. The structure of the calculations that will be performed for case CRA14-0 is listed below.

Parameter Sampling: LHS

Parameter values prescribed to STEEL:CORRMCO2 in a given vector are sampled. As a result, parameter sampling performed in case CRA14-TP will be modified in case CRA14-0 to also include sampling of the refined distributions assigned to parameter STEEL:CORRMCO2. Three replicates of 100 vectors will be created using the computer code LHS. LHS sampling in case CRA14-0 will be done to reflect sampled CRA-2014 PA parameters listed under case CRA14-0 in Table 2-11. Parameter distributions used in the PABC-2009 will be used for sampled parameters not listed under case CRA14-0 in Table 2-11. The random seed and parameter ordering from the PABC-2009 will be used for case CRA14-0 to allow for vector by vector comparison.

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Salado Flow: BRAGFLO

Input files used in case CRA14-BL will be modified for case CRA14-0 so that they include parameters associated with the refinement to the repository water budget implementation discussed in Section 2.1.10. Three BRAGFLO replicates will be executed for case CRA-2014-0, with each replicate consisting of 100 vectors over 6 scenarios (see Table 2-12). The codes PREBRAG version 8.02, BRAGFLO version 6.02, and POSTBRAG version 4.00A will be used for case CRA14-0. PREBRAG version 8.02 and BRAGFLO version 6.02 have been updated and qualified since the PABC-2009 to incorporate a refined repository water balance that includes MgO hydration.

Direct Solids Releases: DRSPALL and CUTTINGS_S

Updates to parameter STEEL:CORRMCO2 and an updated water budget implementation potentially impact repository pressures and brine saturations calculated with BRAGFLO. Spallings release volumes depend directly on repository pressure at the time of intrusion. As parameter refinements included in the CRA-2014 PA potentially impact spallings, as well as cuttings and cavings, releases, three replicates will be executed for case CRA14-0 to determine the impact of changes included in the CRA-2014 PA on direct solids releases.

Actinide Mobilization: PANEL

Code PANEL results for case CRA14-BV utilize the full set of solubilities listed in Table 2-8 for a single replicate. PANEL results obtained in case CRA14-BV will be extended to three replicates in case CRA14-0. The result will be a full set of actinide mobilization results that incorporate all of the radionuclide solubilities listed in Table 2-8.

Salado Transport: NUTS and PANEL

Three replicates of NUTS calculations will be executed for case CRA14-0 to assess the impact of CRA-2014 PA changes on Salado transport results. Changes included in case CRA14-0 potentially alter BRAGFLO results obtained for the E2E1 intrusion combination (BRAGFLO scenario S6-BF). BRAGFLO scenario S6-BF results are used by PA code PANEL (run in "intrusion mode") to calculate radionuclide transport to the Culebra. As a result, three replicates of PANEL_INT calculations will be performed for case CRA14-0 using the same procedure that was used in the PABC-2009 PANEL_INT calculations.

Direct Brine Releases: BRAGFLO

As the changes incorporated into case CRA14-0 potentially impact pressure and brine saturation in waste-containing repository regions, DBR calculations consisting of three replicates will be performed as part of case CRA14-0. Input files used in case CRA14-BL will be modified for case CRA14-0 so that they include parameters associated with the refinement to the repository water budget implementation discussed in Section 2.1.10. Conditions required for the initiation of a DBR release will remain unchanged from the PABC-2009, and the DBR volumes will be

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calculated for the same scenarios and times (see Table 2-13). The codes PREBRAG version 8.02, BRAGFLO version 6.02, and POSTBRAG version 4.00A will be used for case CRA14-0. PREBRAG version 8.02 and BRAGFLO version 6.02 have been updated and qualified since the PABC-2009 to incorporate a refined repository water balance that includes MgO hydration.

CCDF Construction: CCDFGF

Code CCDFGF will be re-run in case CRA14-0 to capture release impacts associated with changes included in the CRA-2014 PA, with results generated for three replicates. Mean CCDFs for each release pathway will be calculated. The 95% confidence limit on the mean will also be calculated. CCDFGF calculations in case CRA14-0 will utilize PANEL actinide mobilization results that correspond to 1x, 2x, 3x, 4x, and 5x the minimum repository brine volume necessary for a DBR.

Sensitivity Analysis: STEPWISE

The CRA-2014 PA will implement sensitivity analyses for results from the major codes. This work falls under the scope of case CRA14-0 as all changes included in the CRA-2014 PA are utilized in that case. Sensitivity analyses will be conducted in a manner consistent with those employed for the PABC-2009. Specifically, global sensitivity analyses will be conducted on the results from CCDFGF using the linear regression code STEPWISE version 2.21.

2.3.2.5 Summary of Code Executions for the CRA-2014 PA

A summary of the codes executed in the CRA-2014 PA is shown in Table 2-14. As discussed in Section 2.3.1, changes included in the CRA-2014 PA are incorporated sequentially in the four cases considered in the CRA-2014 PA. See Table 2-11 for specific changes included in each case.

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Table 2-14: Codes Executed for Cases Considered in the CRA-2014 PA

	CRA-2014 PA Cases			
	CRA14-BL	CRA14-TP	CRA14-BV	CRA14-0
Codes Run	EPAUNI LHS BRAGFLO CUTTINGS_S PANEL (with one brine volume) NUTS BRAGFLO (DBR) CCDFGF (with one brine volume)	LHS CUTTINGS_S CCDFGF (with one brine volume) Results obtained or used in case CRA14-BL will be used for codes not listed above.	PANEL (with five brine volumes) CCDFGF (with five brine volumes) Results obtained or used in case CRA14-TP will be used for codes not listed above.	LHS BRAGFLO CUTTINGS_S PANEL (with five brine volumes) NUTS BRAGFLO (DBR) CCDFGF (with five brine volumes) STEPWISE Case CRA14-0 incorporates all changes included in the CRA-2014 PA.
Number of Replicates	1	1	1	3

2.4 *Reports and Documentation*

Several reports will be generated as a result of this analysis plan. Each set of calculations discussed in Section 2.3 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 PABC-2009 calculations; and
2) analysis of results relevant to the long term performance of the repository. The analysis will include comparisons of CRA-2014 PA results with PABC-2009.

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-2014 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.

Additional analyses, calculations, and documentation performed as part of the regulatory review and approval process for the CRA-2014 PA will also fall under AP-164.

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3 Tasks

The tasks, responsible personnel and estimated task schedule are summarized below in Table 3-1.

Table 3-1: Task List and Estimated Schedule for the CRA-2014 PA

Task	Description	Guiding Document	Approximate Completion Date	Responsible Individual(s)
1	**Preparation Tasks**			
1a	FEPs reassessment	SP 9-4	2/22/13	Kirkes
1b	Inventory Analysis	AP-164	2/13/13	Kicker Zeitler
1c	Solubility Analysis	AP-153	2/18/13	Brush
1d	Drilling Parameter Analysis	AP-164	2/18/13	Camphouse
1e	GLOBAL:PBRINE Analysis	AP-164	2/18/13	Kirchner
1f	STEEL:CORRMCO2 Analysis	AP-159	2/18/13	Roselle
1g	BOREHOLE:TAUFAIL Analysis	AP-163	2/18/13	Herrick
1h	Refined Water Balance Analysis	AP-164	2/18/13	Clayton
2	**Parameter Entry**			
2a	Inventory Parameters	SP 9-5	2/18/13	Long
2b	Solubility Parameters	SP 9-5	2/18/13	Long
2c	Drilling Parameters	SP 9-5	2/19/13	Long
2d	Water Balance Parameters	SP 9-5	2/19/13	Long
2e	Other Parameters	SP 9-5	2/20/13	Long
3	**Code Run Environment Preparation**			
3a	Libraries Update	AP-164	2/21/13	Long
3b	Run Control Script Update	AP-164	4/9/13	Long
4	**Calculation Preparation**			
4a	Input Files Prepared	AP-164	2/20/13	Camphouse Kicker Kim Kirchner Malama Zeitler
4b	Input Files Reviewed	AP-164	2/21/13	Camphouse
5	**Calculations (Case CRA14-BL)**			
5a	Parameter Sampling: LHS	AP-164	2/22/13	Long
5b	Salado Flow: BRAGFLO	AP-164	2/26/13	Long
5c	Cuttings & Cavings: CUTTINGS_S	AP-164	2/27/13	Long
5d	Direct Brine Releases: BRAGFLO	AP-164	3/1/13	Long
5e	Actinide Mobilization: PANEL	AP-164	3/4/13	Long
5f	Salado Transport: NUTS & PANEL	AP-164	3/7/13	Long
5g	Solid Normalized Release: EPAUNI	AP-164	3/8/13	Long
5h	CCDF Construction: CCDFGF	AP-164	3/11/13	Long
6	**Calculations (Case CRA14-TP)**			
6a	Parameter Sampling: LHS	AP-164	3/12/13	Long

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6b	Cuttings & Cavings: CUTTINGS_S	AP-164	3/13/13	Long
6c	CCDF Construction: CCDFGF	AP-164	3/13/13	Long
7	**Calculations (Case CRA14-BV)**			
7a	Actinide Mobilization: PANEL	AP-164	3/14/13	Long
7b	CCDF Construction: CCDFGF	AP-164	3/15/13	Long
8	**Calculations (Case CRA14-0)**			
8a	Parameter Sampling: LHS	AP-164	3/18/13	Long
8b	Salado Flow: BRAGFLO	AP-164	3/22/13	Long
8c	Cuttings & Cavings: CUTTINGS_S	AP-164	3/25/13	Long
8d	Direct Brine Releases: BRAGFLO	AP-164	3/29/13	Long
8e	Actinide Mobilization: PANEL	AP-164	4/1/13	Long
8f	Salado Transport: NUTS & PANEL	AP-164	4/5/13	Long
8h	CCDF Construction: CCDFGF	AP-164	4/8/13	Long
8i	Sensitivity Analysis: STEPWISE	AP-164	4/9/13	Long
9	**Analysis & Documentation**			
9a	Inventory Analysis Report	AP-164	2/18/13	Kicker Zeitler
9b	FEPs Re-assessment	SP 9-4	5/31/13	Kirkes
9c	Parameter Sampling: LHS	AP-164	4/22/13	Kirchner
9d	Salado Flow: BRAGFLO	AP-164	4/26/13	Camphouse
9e	Cuttings & Cavings: CUTTINGS_S	AP-164	4/29/13	Kicker
9f	Direct Brine Releases: BRAGFLO	AP-164	5/3/13	Malama
9g	Actinide Mobilization: PANEL	AP-164	5/6/13	Kim
9h	Salado Transport: NUTS & PANEL	AP-164	5/10/13	Kim
9i	Solid Normalized Releases: EPAUNI	AP-164	5/10/13	Kicker
9j	CCDF Construction: CCDFGF	AP-164	5/13/13	Zeitler
9k	Sensitivity Analysis: STEPWISE	AP-164	5/15/13	Kirchner
9l	Run Control Document	AP-164	5/15/13	Long
9m	Summary Report	AP-164	5/31/13	Camphouse

4 Software

The major WIPP PA codes to be used for this analysis are listed in Table 4-1. These codes will be executed on the WIPP PA Alpha Cluster, which is listed in Table 4-2. Additionally, COTS software, such as MATHEMATICA®, MATLAB®, MATHCAD®, Excel®, Access®, Grapher®, or Kaleidagraph® may be utilized. The use of any COTS application will be verified per NP 9-1 Appendix C as appropriate.

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Table 4-1: Codes to be used for the CRA-2014 PA.

Code	Version	Executable	Build Date
ALGEBRACDB	2.35	ALGEBRACDB_PA96.EXE	31-01-96
BRAGFLO (for case CRA14-BL)	6.0	BRAGFLO_QB0600.EXE	12-02-07
BRAGFLO (for case CRA14-0)	6.02	BRAGFLO_QB0602.EXE	11-29-12
CCDFGF	6.0	CCDFGF_QC0600.EXE	02-23-10
CUTTINGS_S	6.02	CUTTINGS_S_QA0602.EXE	09-06-05
EPAUNI	1.15A	EPAUNI_QA0115A.EXE	07-03-03
GENMESH	6.08	GM_PA96.EXE	31-01-96
ICSET	2.22	ICSET_PA96.EXE	01-02-96
LHS	2.42	LHS_QA0242.EXE	18-01-05
MATSET	9.20	MATSET_QA0920.EXE	04-01-12
NUTS	2.05C	NUTS_QA0205C.EXE	05-24-06
PANEL	4.03	PANEL_QA0403.EXE	04-25-05
PCCSRC	2.21	PCCSRC_PA96.EXE	05-23-96
POSTBRAG	4.00A	POSTBRAG_QA0400A.EXE	28-03-07
POSTLHS	4.07A	POSTLHS_QA0407A.EXE	25-04-05
PREBRAG (for case CRA14-BL)	8.00	PREBRAG_QA0800.EXE	08-03-07
PREBRAG (for case CRA14-0)	8.02	PREBRAG_QA0802.EXE	11-29-12
PRECCDFGF	2.0	PRECCDFGF_QA0200.EXE	04-06-10
PRELHS	2.40	PRELHS_QA0240.EXE	04-01-12
RELATE	1.43	RELATE_PA96.EXE	06-03-96
STEPWISE	2.21	STEPWISE_PA96_2.EXE	02-12-96
SUMMARIZE	3.01	SUMMARIZE_QB0301.EXE	21-12-05

Table 4-2: 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

None

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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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