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TECHNICAL SUPPORT DOCUMENT FOR SECTION 194.23

REVIEW OF THE 2009 COMPLIANCE RECERTIFICATION
PERFORMANCE ASSESSMENT BASELINE CALCULATION
(PABC-2009)

U. S. ENVIRONMENTAL PROTECTION AGENCY
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ACRONYM LIST

ATWIR	Annual Transuranic Waste Inventory Report
BL	Babock and Wilcox
CARD	Compliance Application Review Document
CCA	Compliance Certification Application
CDB	Post-processed binary file
CDF	Cumulative distribution function
CCDF	Complementary cumulative density function
CFR	*Code of Federal Regulations*
CID	Comprehensive Inventory Database
CH	Contact-handled
Ci	Curies
CO_2	Carbon dioxide
CPR	Cellulosics, plastics and rubber
CRA	Compliance Recertification Application
D	Difference between log values of measured and calculated solubilities
DBR	Direct brine release
DOE	U.S. Department of Energy
DRZ	Disturbed Rock Zone
EDTA	Ethylenediaminetetraacetic acid
EPA	U.S. Environmental Protection Agency
FEPs	Features, events, and processes
FMT	Fracture Matrix Transport
GE-VNC	General Electric - Vallecitos Nuclear Center
GWB	Generic Weep Brine
INL	Idaho National Laboratory
K_ds	Distribution coefficient
LANL	Los Alamos National Laboratory
LANL-CO	Los Alamos National Laboratory – Carlsbad Operations
LHS	Latin Hypercube Sampling
LLNL	Lawrence Livermore National Laboratory
LWA	Land Withdrawal Act

LWB	Land Withdrawal Boundary
m	Molal (moles/kg)
M	Molar (moles/liter)
MFC	Material Fuel Complex
MB	Marker Bed
MgO	Magnesium oxide
MPa	Megapascal
NRD	Nuclear Radiation Development
ORNL	Oak Ridge National Laboratory
PA	Performance assessment
Pa	Pascal
PABC	Performance Assessment Baseline Calculation
PAIR	Performance Assessment Inventory Report
PAPDB	Performance Assessment Parameter Database
PAVT	Performance Assessment Verification Testing
pcH	Negative log of the hydrogen ion concentration, molar units
PCR	Planned Change Request
pH	Negative log of the hydrogen ion activity
QA	Quality Assurance
RCHCM	Culebra hydrology conceptual model
RFETS	Rocky Flats Environmental Technology Site
RH	Remote-handled
RL	Hanford Richland
RP	River Protection (Hanford Office of)
S_M	Measured solubility
S_P	Predicted solubility
SNL	Sandia National Laboratories
SO-C	Screened out on the basis of low consequence
SO-R	Screened out on a regular basis
SQS	Small quantity site
SRRC	Standardized rank regression coefficient
SRS	Savannah River Site
T	Transmissivity

TBM	Technical Baseline Migration
TDOP	Ten-drum overpack
TRU	Transuranic
TSD	Technical Support Document
TWBID	Transuranic Waste Baseline Inventory Database
TWBIR	Transuranic Waste Baseline Inventory Report
V	Volume
WIPP	Waste Isolation Pilot Plant
WM	Waste material
WMP	Waste Material Parameter
WSDT	Working Site Data Template
WTWBIR	WIPP Transuranic Waste Baseline Inventory Report
WWIS	WIPP Waste Information System

EXECUTIVE SUMMARY

The U.S. Department of Energy (DOE) operates the Waste Isolation Pilot Plant (WIPP) for the disposal of defense-related transuranic (TRU) waste. DOE submitted the Compliance Certification Application (CCA) to the U.S. Environmental Protection Agency (EPA or the Agency) in 1996. As required by 40 CFR § 194.34, the CCA included the results of a performance assessment (the CCA PA) carried out to predict the ability of the repository to meet the regulatory containment requirements. After review of the CCA documentation and the CCA PA results, the Agency required that DOE perform a revised PA, referred to as the Performance Assessment Verification Testing (PAVT). The results of the PAVT and review of the CCA and supplemental information formed the basis of the Agency's certification that DOE had met the appropriate regulatory requirements. WIPP began accepting waste in March 1999.

DOE is required to submit a Compliance Recertification Application (CRA) every 5 years after the date waste was first received at WIPP; the first CRA (CRA-2004) was submitted in March 2004 (DOE 2004b). CRA-2004 was based on a PA that included revisions since the PAVT. After review of CRA-2004 and additional information provided by DOE, the Agency found that changes would be required to the CRA-2004 PA (EPA 2005a). Consequently, DOE prepared a new PA, referred to as the Performance Assessment Baseline Calculation (PABC-2004 or PABC04) (EPA 2006c). The PABC-2004 assumptions, parameters, calculations and results were reviewed by the Agency, and this PA formed the basis of EPA's initial recertification of the WIPP.

DOE submitted its second recertification application designated CRA-2009 in March 2009. On May 21, 2009, EPA informed DOE that a revised PA (referred to here as PABC-2009 or PABC09) would be required before the CRA-2009 could be judged to be complete (Cotsworth 2009a). This report represents EPA's assessment and evaluation of the PABC-2009 results. The report focuses on those aspects of PA that are significantly different from the PABC-2004.

Section 1 of this report provides a brief introduction to WIPP, the PABC-2009 and prior PAs.

In Section 2, the features, events and processes (FEPs) that were identified and included in the CRA-2004 PA were reassessed by DOE for the CRA-2009 PA and again for the PABC-2009. A total of 57 FEPs were changed or updated by DOE between the CRA-2004 PA and the CRA-2009 PA. No FEPs were deleted during this period, and 188 of the 235 FEPs considered for the CRA-2004 PA remained unchanged. With the addition of 10 new FEPs, a total of 245 FEPs were considered for the CRA-2009 PA. None of the screening arguments or name changes resulted in screening decision changes. As part of the preparatory activities for the PABC-2009, DOE again examined the FEPs to determine if the FEPs baseline remained valid in consideration of the changes that occurred since the CRA-2009 data cutoff. This assessment determined that the FEPs baseline remained valid, because the changes in parameter values in the PABC-2009 did not affect FEP identifications, screening arguments or screening decisions. No newly created FEPs were required, and no changes were needed in the FEP baseline.

Section 3 describes the inventory used in the PABC-2009. The DOE used the PABC-2004 inventory to develop the inventory for the CRA-2009 PA. This inventory was carefully reviewed and validated by EPA in its previous recertification decision. The PABC-2009 used

the Performance Assessment Inventory Report (PAIR) – 2008, which documented the waste inventory as of December 31, 2007. During the course of its review of the PABC-2009, EPA examined the quality assurance (QA) procedures used to populate the Comprehensive Inventory Database (CID), to update the CID annually, and to transfer data from the WIPP Waste Information System (WWIS) to the CID. In addition, procedures used to verify chemical components in the waste and estimate the quantities in the waste were reviewed. Spot checks were made of various calculated values in the inventory documentation, and the checked values were determined to be correct. EPA audited radioactive decay calculations and demonstrated good agreement between the Agency's calculations and the values reported by DOE. EPA also determined that DOE had adequately responded to CRA-2009/PABC-2009 completeness comments related to inventory. On the basis of its review, EPA concluded that DOE has appropriate QA procedures in place to accurately document the WIPP waste inventory on an annual basis. EPA further concluded that the PAIR 2008 inventory is appropriate for use in PA calculations.

DOE must demonstrate that PA software is in compliance with regulatory requirements of 40 CFR § 194.23. Section 4 describes the Agency's review of DOE's testing of the PA computer codes to show that they perform properly on the updated hardware and software implemented since the PABC-2004. Based on its review, the Agency concluded that the PA codes and designated systems are approved for use in compliance calculations.

Section 5 describes the Agency's review of changes in the WIPP parameter database since the PABC-2004. The Agency's review occurred in two stages, consistent with DOE's preparation of the CRA-2009 PA and the PABC-2009 PA. The Agency assessed the transcription accuracy, documentation, and traceability of changes to the parameter values and metadata that have occurred since the PABC-2004, as well as the retrievability of supporting documents and the database-code interface accuracy. The procedural adequacy of changes made to the database and the technical adequacy of all database changes were also reviewed. The results of these reviews indicated that the parameters used in the PABC-2009 PA were technically acceptable and appropriately documented.

Anoxic corrosion of metals and microbial degradation of cellulosics, plastics and rubber (CPR) may influence WIPP repository performance because of their effects on repository chemistry and gas generation. Section 6 describes the results of the Agency's review of these processes. The conceptual model and implementation of gas generation from anoxic corrosion used for the PABC09 continue to be supported by the available data. The microbial gas generation rates used for the PABC09 are appropriate for modeling gas generation rates from degradation of cellulosic materials, but may overestimate gas generation rates from the degradation of plastics and rubber. DOE accounted for uncertainties regarding the rates of plastic and rubber degradation in the WIPP repository environment by assuming plastic and rubber degradation occurs in only 25% of the realizations. Based on the available data, the approach for modeling microbial gas generation rates was appropriate for the PABC09.

Actinide mobilization and the development of uncertainty distributions for actinide solubilities are reviewed in Section 7. The available data support the assumption that the magnesium oxide (MgO) backfill will adequately control brine pH and carbon dioxide (CO_2) fugacities, and thereby limit actinide solubilities in WIPP brines under inundated conditions. The assumptions

related to actinide oxidation states in the WIPP repository have remained unchanged since they were developed and peer reviewed for the CCA. It is assumed that thorium(IV), americium(III), and curium(III) are the only oxidation states that will be present in the WIPP repository for these radionuclides. It is assumed that plutonium may be present in the +III or +IV oxidation states, neptunium may be present in the +IV or +V oxidation states, and uranium may be present in the +IV or +VI oxidation states. Because of the reducing conditions that will be established in the repository shortly after closure, these oxidation state assumptions are appropriate for the PABC09.

DOE provided a qualitative review of actinide solubility and speciation data relevant to WIPP brines that became available since the PABC04, but did not revise the FMT database for the PABC09 actinide solubility calculations. EPA reviewed the actinide solubility and aqueous speciation data that have become available since the most recent revision of the FMT database, and determined that the actinide solubilities calculated using this database were adequate for use in the PABC09. EPA also reviewed the development of the +III and +IV actinide solubility uncertainty distributions and the colloidal actinide source term calculations and determined that these calculations were also adequate for the PABC09.

In the PABC-2009 as in previous PAs, the Culebra member of the Rustler Formation is conceptualized as a horizontal, confined aquifer of uniform density. For fluid flow, the Culebra is assumed to be a heterogeneous porous medium with spatially varying transmissivity. A heterogeneous velocity field is also assumed to be used for radionuclide transport, but all other rock properties are conceptualized as constant (homogeneous) across the model area. The Culebra is assumed to have two types of porosity; a portion of the porosity is associated with high-permeability features, where transport occurs by advection, and the rest of the porosity is associated with low-permeability features, where flow does not occur and retardation occurs by physical processes (diffusion) and chemical processes (sorption).

The key factors controlling fluid flow in the Culebra are the hydraulic gradient, transmissivity distribution and porosity. In the Culebra conceptual model, the spatial distribution of transmissivity is important. The hydraulic gradient and transmissivities used in PA are coupled, because they are calibrated to observed conditions. If radionuclides are introduced into the Culebra, they may be transported from the point of introduction by groundwater flowing naturally through the Culebra.

Many additional Culebra transmissivity datasets are now available, compared with the information utilized to generate the transmissivity fields (T-fields) used in the CRA-2009 PA (Beauheim 2010). Additional locations near the WIPP site have been tested and long-term pumping tests have been performed. The additional datasets and modified conceptual model were used for the PABC-2009 T-field calibration. This modified conceptual model was peer reviewed and determined to be appropriate for calculating transmissivity field within the Culebra.

Section 9 describes EPA's evaluation of distribution coefficients (K_ds) used for flow and transport modeling in the Culebra. Radionuclides may reach the Culebra member of the Rustler Formation via brine flow through a borehole that intersects the repository. These radionuclides

may then be transported by groundwater flow to the accessible environment. Predictions of transport and release of radionuclides through the Culebra are affected by sorption onto minerals along this potential pathway. Accordingly, DOE developed K_ds to express a linear relationship between sorbed and aqueous concentrations of the radionuclides.

Based on the current waste inventory, higher organic ligand concentrations have been predicted for the PABC-2009 than for previous PAs. Consequently, DOE re-evaluated the range of K_d values used to assess retardation of actinides during transport through the Culebra. There was no evidence indicating that the upper bound should be changed. However, the lower bounds were reduced to account for the possibility of higher organic ligand concentrations. The revised lower-bound values for the K_ds used in the PABC-2009 are consistent with the lower limits of the ranges observed in the experiments with high concentrations of organic ligands. Based on its review, EPA determined that the K_d ranges were appropriate for use in the PABC-2009.

Section 10 describes the Agency's review of the Salado flow and transport modeling. Flow in the Salado is computed by the BRAGFLO code, which simulates brine and gas flow in and around the repository. BRAGFLO includes the effects of processes such as gas generation and creep closure. Outputs from the BRAGFLO simulations describe the conditions (pressure, brine saturation, porosity) and flow patterns (brine flow up an intrusion borehole and out anhydrite marker beds to the accessible environment) that are used by other software to predict radionuclide releases.

Changes in the CRA-2009 BRAGFLO analysis from the PABC-2004 BRAGFLO analysis included:

(1) Additional CPR inventory, due to the emplacement materials
(2) Slightly higher halite and DRZ porosity
(3) Slight modification to the way in which the humid CPR degredation rate is calculated
(4) Change to the way in which the effective saturation is calculated at low saturations
(5) Additional smoothing to chemical reaction rates
(6) New capillary-pressure model for open cavities

EPA required that the DOE revise the CRA-2009 PA analysis and present the new results before the Agency would judge the CRA-2009 to be complete (Cotsworth 2009a). Between the CRA-2009 PA and the PABC-2009 analysis, there are two sets of parameter changes that have a significant impact on Salado transport. The CRA-2009 PA used the waste inventory from the CRA-2004 PABC; this has since been updated, and the most recent inventory report has been used. Among the changes to the inventory was a redistribution in the relative amounts of different isotopes in the repository, which will lead to changes in potential releases as a result of the different half-lives of different waste components. The net increase in the total inventory of the repository that contributes to the Waste Unit Factor (WUF), from 2.32 MCi to 2.6 MCi, is not expected to cause a significant change in behavior, as the definition of EPA units for releases takes the total inventory of the repository into account. In a separate change, the probability distribution for the baseline solubility limit for +III and +IV actinides has been revised. The new distributions for the solubility limits change the amount of actinides that can be dissolved into any brine that may be present, and consequently the amount of actinides that can reach the surface or the Land Withdrawal Boundary (LWB).

The Agency has concluded that changes to the computer codes for modeling Salado Formation flow and transport have been properly implemented, as have changes in conceptual models and model parameters. The Agency finds that the approach taken by DOE for modeling the Salado is acceptable.

In Section 11, the PABC-2009 direct-release calculations are reviewed and the results compared to those obtained for the PABC-2004. Direct releases are defined as solid and liquid materials removed from the repository and carried to the ground surface through intrusion boreholes at the time of drilling. Direct releases occur in WIPP PA through cuttings and cavings releases, direct brine releases (DBRs) and spallings releases. Cuttings and cavings are the solid materials removed from the repository and carried to the ground surface by drilling fluid during the process of drilling a borehole that intersects the repository. Cuttings are the materials removed directly by the drill bit, and cavings are the materials eroded from the borehole walls by shear stresses from the circulating drilling fluid. The contribution of mean cuttings and cavings releases to total mean radionuclide releases for the PABC-2009 PA remained essentially unchanged from the PABC-2004 PA. Direct brine releases occur when contaminated brine originating in the repository is driven up an intrusion borehole to the ground surface by repository gas pressures that exceed the estimated 8 MPa hydrostatic pressure of the drilling fluid. Because of a combination of increased actinide solubilities (Section 7.0) and higher repository gas pressures (Section 6.0), the contribution of DBR to total mean direct radionuclide releases for the PABC-2009 PA was greater than for the PABC-2004 PA at all probabilities of occurrence. Spallings releases occur when solid waste is ejected through an intrusion borehole by repository gas pressures that exceed the 8 MPa hydrostatic pressure of the drilling fluid and cause tensile failure of the waste. Spallings releases calculated for the PABC-2009 PA increased at higher probabilities of occurrence as compared with the PABC-2004 PA. This increase in spallings releases was caused primarily by the increase in repository gas pressure.

Section 12 describes the Agency's review of the results of total normalized releases, including releases through both undisturbed and disturbed pathways. Normalized releases calculated for the PABC-2009 are summarized and the sensitivity analyses of the results are reviewed. Total normalized releases are calculated by totaling the releases from each pathway and primarily consist of cuttings and cavings releases, DBRs, spallings releases and releases from the Culebra. There were no releases from transport up the shaft in the PABC-2009 and no significant disturbed releases through the anhydrite interbeds. Undisturbed releases through the anhydrite interbeds in the PABC-2009 were as much as 11 orders of magnitude smaller than the typical disturbed releases, and therefore were not significant contributors to total normalized releases.

Because cuttings, cavings, direct brine and spallings releases account for an overwhelming majority of the total releases, the calculated total releases are most sensitive to uncertainties in the parameters governing these release mechanisms. In both the PABC-2004 and the PABC-2009 analyses, total normalized releases were most sensitive to uncertainty in waste shear strength (WTAUFAIL), which is a key parameter governing the volume of cavings. In the PABC-2009, direct brine releases are the second most important contributor to total releases, and even surpass cuttings and cavings at low probabilities. Consonant with this, the second most important variable in the PABC-2009 analysis is WSOLVAR3, a solubility multiplier representing uncertainty in solubilities for all actinides in the +3 oxidation state. These two parameters account for 79% of the uncertainty in total normalized releases.

Section 13 provides a summary and the conclusions of the Agency's review of PABC-2009. Based on the information presented in this report, EPA believes that the revised PA (PABC-2009) contains all of changes requested by the Agency. These changes are transparent, traceable against prior PAs, consistent with EPA direction, and appear to be properly implemented. DOE has answered all comments on the CRA-2009 and the PABC-2009 to EPA's satisfaction. The PABC-2009 results described in Section 12 show that the WIPP continues to comply with the containment requirements of 40 CFR § 191.13.

1.0   INTRODUCTION

The U.S. Department of Energy (DOE) operates the Waste Isolation Pilot Plant (WIPP) for the disposal of defense-related transuranic (TRU) waste. DOE submitted the Compliance Certification Application (CCA) to the U.S. Environmental Protection Agency (EPA or the Agency) in 1996. As required by 40 CFR § 194.34, the CCA included the results of a performance assessment (the CCA PA) carried out to predict the ability of the repository to meet the containment requirements. After review of the CCA documentation and the CCA PA results, the Agency required that DOE perform a revised PA, referred to as the Performance Assessment Verification Testing (PAVT). The results of the PAVT and review of the CCA and supplemental information formed the basis of the Agency's certification that DOE had met regulatory requirements. WIPP began accepting waste in March 1999.

DOE is required to submit a Compliance Recertification Application (CRA) every 5 years after the date waste was initially received at WIPP; the first CRA (CRA-2004) was submitted in March 2004 (DOE 2004b). After review of the CRA-2004 and additional information provided by DOE, the Agency found that changes would be required to the PA (EPA 2005a). Consequently, DOE carried out a new PA,[1] referred to as the Performance Assessment Baseline Calculation (PABC-2004 or PABC04). Acceptability of this PA was a significant factor in EPA's 2006 compliance recertification.

DOE submitted its second recertification application designated CRA-2009 in March 2009. On May 21, 2009, EPA informed DOE that a revised PA (referred to here as PABC-2009 or PABC09) would be required before the CRA-2009 could be judged to be complete (Cotsworth 2009a). This report represents EPA's assessment and evaluation of the PABC-2009 results. The report focuses on those aspects of the PA that are significantly different from the PABC-2004.

In Section 2 of this report, the features, events, and processes (FEPs) identified and included in the CCA PA (DOE 1996b) and PABC-2004 are reassessed for PABC-2009. Section 3 describes the inventory used in the PABC-2009 calculations. Section 4 describes the Agency's review of the PA computer codes to show that they perform properly on the updated hardware and software implemented since PABC-2004. Section 5 describes the Agency's review of changes in the WIPP parameter database since the PABC-2004.

Section 6 presents the results of the Agency's review of the effects of anoxic corrosion of metals and microbial degradation of cellulosics, plastics and rubber (CPR) on repository chemistry and gas generation. Actinide solubility calculations and the development of uncertainty distributions for actinide solubilities are reviewed in Section 7. Section 8.0 describes the Agency's review of the Culebra flow and transport modeling, while information on distribution coefficients used in flow and transport modeling is presented in Section 9. Section 10 describes a related review of the Salado flow and transport modeling.

In Section 11, the PABC-2009 direct-release calculations are reviewed and the results compared to those obtained for the PABC-2004. Section 12 describes the Agency's review of the summary

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[1] DOE documents refer to the PABC as the CRA-2004 PABC. For simplicity and clarity, EPA has chosen the shorter description used here.

results of the PABC-2009, including releases through undisturbed pathways and disturbed pathways. Finally, Section 13 summarizes the Agency's conclusions regarding the acceptability of the PABC-2009 in determining continuing compliance with 40 CFR Part § 194.34.

This report presents EPA's review of the major elements used to develop the inputs to the PABC-2009 and the results of the PA calculations. The review provides the basis for EPA conclusions regarding the acceptability of the PABC-2009 as one of the bases for compliance recertification. Individual Technical Support Douments (TSDs) have been prepared covering parameters, FEPs, human intrusion, waste inventory, models and codes, and repository chemistry (EPA 2010a, EPA 2010b, EPA 2010c, EPA 2010d, EPA 2010e, EPA 2010f). While each of these topics is discussed here, the reader is referred to specific TSDs for additional details.

2.0 FEPS REVIEW

The FEPs that were identified and included in the CRA-2004 PA (DOE 2004b, Appendix PA, Attachment SCR) were reassessed by DOE for the CRA-2009 PA (DOE 2009, Appendix SCR) and again for the PABC-2009 (Clayton et al. 2010). These reassessments were required by 40 CFR § 194.15(a). DOE's FEPs reassessment process, procedurally documented in Kirkes 2009a, focused primarily on updating FEP screening arguments as a result of changes in the PA models and new information obtained since the CRA-2004 PA. The following changes were made in the FEPs baseline developed for the CRA-2009 PA (Kirkes 2008):

- The screening decision for one FEP (H41: Human-induced surface disruptions) was changed from SO-R (screened out on a regulatory basis) to SO-C (screened out on the basis of low consequence) to correct an inconsistency identified in the Agency's CRA-2004 FEPs review. As noted, this FEP remained "screened-out" and was therefore not incorporated into the CRA-2009 PA.

- The screening argument for one FEP (N40: Impact of a large meteorite) was changed to correct an error in impact frequency discovered during DOE's review.

- The names were changed for 10 existing FEPs and 10 new FEPs were created to better distinguish between activities inside and outside the WIPP land withdrawal boundary, and between panel closure seals and shaft seals.

- Screening arguments for 35 FEPs were updated with new information associated with relevant features and processes, such as seismic activity, drilling rates, new wells and mining activities.

A total of 57 FEPs were changed or updated by DOE between the CRA-2004 PA and the CRA-2009 PA. No FEPs were deleted during this period, and 188 of the 235 FEPs considered for the CRA-2004 PA remained unchanged. With the addition of 10 new FEPs, a total of 245 FEPs were considered for the CRA-2009 PA. None of the screening arguments or name changes resulted in screening decision changes.

Following its technical review of the CRA-2009 PA, the Agency requested that additional information received by DOE between the data cutoff for the CRA-2009 PA (December 2007) and the submittal of CRA-2009 (March 2009) be included in an additional PA calculation designated the PABC-2009. This new information included updated waste inventory, actinide solubilities and uncertainties, matrix partition coefficients (K_ds), Culebra transmissivity fields and drilling parameters. DOE performed an assessment of the FEPs baseline that had been developed for the CRA-2009 PA (Kirkes 2009b) as part of the preparatory activities for the PABC-2009 to determine if the FEPs baseline remained valid in consideration of the changes that occurred since the CRA-2009 data cutoff. This assessment determined that the FEPs baseline remained valid, because the changes in parameter values in the PABC-2009 did not affect FEP identifications, screening arguments or screening decisions. No newly created FEPs, therefore, were required, and no changes were needed in the FEP baseline.

DOE's methodology for dealing with the potential impacts of changes in FEPs or changes in PA calculations is documented in the new Sandia National Laboratories (SNL) Activity Specific

Procedure SP 9-4, *Performing FEPs Baseline Impact Assessment for Planned or Unplanned Changes* (Revision 2) (Kirkes 2009a). This procedure was written to help assure that the FEPs baseline is managed and updated systematically over time, rather than updated only immediately prior to recertification.

The process for updating the FEPs baseline begins by obtaining the most recent version of the Baseline FEPs List from the SNL Records Center in Carlsbad, New Mexico. The nature and scope of the PA changes are compared with the current, updated FEPs baseline, and all related FEPs are identified. The need for new FEPs is determined, and those are added to the baseline in accordance with NP 6-1, *Document Review Process* (Chavez 2008). Screening arguments and decisions are modified for existing FEPs as needed, and additional activities, such as the need to develop new or revised process models, are identified. The results of this Baseline FEPs Assessment are then documented in an appropriate analysis report following NP 6-1 and NP 17-1, *Records* (Sosa 2006), as appropriate. The PA Manager is informed of any additional activities affecting PA that are identified, as documented by the mandatory signature of the PA Manager on the FEPs Impact Assessment Report cover sheet.

The major part of the FEPs impact assessment involved an evaluation of each of the changed FEPs that had previously been screened out from PA, to determine whether the screening decision remained valid. As previously noted, none of the changes resulted in screening decision changes.

In summary, DOE's FEPs impact assessment did not identify any inconsistencies or omissions to the current FEPs baseline list as a result of the changes incorporated in the PABC-2009. Further, DOE's assessment did not identify any changes in PA methodology that would be needed to address the FEP updates or changes in screening decisions. The Agency has reviewed the FEP updates and changes, as well as the changes in the PA database and methodology that have occurred since the CRA-2004 PA, and has found DOE's conclusions to be reasonable. A detailed description of the FEP changes and the Agency's evaluation of those changes is presented in EPA 2010d. DOE's evaluation of the FEPs impact assessment, and DOE's conclusion that there are no inconsistencies or omissions between the PABC-2009 PA and the supporting baseline FEPs list, therefore, are warranted and technically valid.

3.0   BASELINE INVENTORY FOR PERFORMANCE ASSESSMENT

This section describes and discusses the inventory used in the PABC-2009. Additional details on EPA's review of the WIPP baseline inventory are presented in *Technical Support Document for Section 194.24: Review of the Baseline Inventory Used in the Compliance Recertification Application (CRA-2009) and the Performance Assessment Baseline Calculation (PABC-2009)* (EPA 2010a).

3.1   EVOLUTION OF THE BASELINE INVENTORY

The first DOE attempt to describe all TRU waste at the waste stream level was documented in the *WIPP Transuranic Waste Baseline Inventory Report* (WTWBIR, Revision 0) issued in June 1994 (DOE 1994). A revised report (WTWBIR, Revision 1) was issued in February 1995 (DOE 1995a). Revision 1 contained modifications based on site reviews and data quality checks. In Revision 2 of the report (DOE 1995b), the title was changed to *Transuranic Waste Baseline Inventory Report* (TWBIR, Revision 2) to reflect the fact that the revision included information on TRU waste not intended for disposal at the WIPP. The June 1996 revision of this report (TWBIR, Revision 3), together with Revision 2, were used by DOE to prepare the CCA. Based on its review of the CCA as submitted by DOE, EPA required DOE to revise some of the parameters and assumptions used in the CCA PA and rerun the PA. This revised PA, the PAVT, was used in May 1998 by EPA to certify that the WIPP meets the disposal standards set forth in 40 CFR Part 191 and the specific WIPP compliance criteria set forth in 40 CFR Part 194. The inventory used for the PAVT calculations was the same as for the CCA PA.

To prepare for its submittal of the CRA-2004, DOE updated the inventory to be current as of September 30, 2002. This revised inventory was documented in Appendix DATA, Attachment F, of the CRA-2004, also referred to by DOE as the *2003 Update Report*.[2] Based on its review of the completeness of the CRA-2004, EPA determined that changes should be made to the PA. Many of these changes were based on errors in the CRA-2004 inventory and changes in assumptions that had occurred since September 30, 2002. This revised PA, designated the PABC-2004, provided the basis for the EPA's initial compliance recertification decision.

The waste inventory used to develop the radionuclide source term for the PABC-2004 was based on information contained in Leigh et al. 2005b. The PABC-2004 inventory was subsequently documented in greater detail in the *Transuranic Waste Baseline Inventory Report – 2004*, referred to here as TWBIR 2004 (DOE 2006). In addition, CPR used in emplacement materials were included in the inventory for the first time. Details on the changes made to develop the PABC-2004 inventory from the CRA-2004 inventory are provided in Leigh et al. 2005b.

The CRA-2004 and the PABC-2004 inventories were thoroughly reviewed by EPA in support of its 2006 recertification decision that the WIPP could continue to accept TRU waste for disposal. EPA documented the results of its inventory review in the Compliance Application Review

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[2] As will be discussed subsequently in this report, inventory information is also located in other sections of the CRA.

Document (CARD) for § 194.24 – Waste Characterization (EPA 2006a) and in the Inventory TSD (EPA 2006b).

The DOE 2009 Compliance Recertification Application used the PABC-2004 inventory as the data source for the CRA-2009 PA. Since this inventory was carefully reviewed and validated by EPA in its previous recertification decision, it will not be reconsidered here, except for comparative purposes. The conclusion from EPA 2006b (pg. 44) is restated for the record:

> *The inventory reported in the* [2004] *CRA, as amended by the* [2004] *PABC, adequately describes the chemical, radiological, and physical composition of the existing and to-be-generated waste as required by 40 CFR 194.24(a). The descriptions provided in the inventory documents reviewed here include comprehensive lists of waste components and their approximate quantities in the waste also required by 40 CFR 194.24(a).*

Since the 2006 compliance decision, four additional inventory reports have been issued by DOE. The TWBIR 2004 documents the PABC-2004 inventory from Leigh et al. (2005b) in greater detail (DOE 2006). The *Annual Transuranic Waste Inventory Report – 2007* (DOE/TRU-2008-3379, Rev.1), revised in mid-2008, presents the status of the inventory as of December 31, 2006, with corrections after that date. The *Annual Transuranic Waste Inventory Report –2008* (DOE/TRU-2008-3425, Rev. 0), published in October 2008, presents the status of the inventory as of December 31, 2007. These documents will be referred to here as ATWIR 2007 and ATWIR 2008.

Since EPA required a new PA to support the 2009 compliance recertification application, DOE proposed that the stand-alone ATWIR 2008 inventory report be used for the PABC-2009, as outlined in the Executive Summary (pg. 5) of ATWIR 2007. The Performance Assessment Inventory Report (PAIR) – 2008 (PAIR 2008) documents the scaling of the data in ATWIR 2008 and provides additional inventory information specific to PA that was not included in ATWIR 2008. A summary of inventory reports and their utilization in various compliance certification/recertification activities is presented in Table 3-1.

Table 3-1.   Sources of Inventory Information for WIPP Certification/Recertifications

Certification/Recertification	Inventory Report Used
CCA	TWBIR, Revisions 2 and 3
CRA-2004	CRA 2004, Appendix DATA, Attachment F
PABC-2004	Leigh et al. 2005b
CRA-2009	Leigh et al. 2005b/TWBIR 2004
PABC-2009	ATWIR 2008/PAIR 2008

3.2   MANAGEMENT OF WIPP INVENTORY DATABASE

The data from which the information in these inventory reports was developed was originally contained in the Transuranic Waste Baseline Inventory Database (TWBID)—a qualified electronic database. A Microsoft Access® 2.0 format database (TWBIR.mdb, dated January 29, 1996) was used to generate TWBIR Revision 3. After compliance certification, this database was converted to Microsoft Access 2000 format and was modified to incorporate new requirements (Appendix DATA, Attachment F, Section DATA-F-2.2.1). This database was named TWBID Revision 2.1. New site data reflective of the then-current TRU inventory status were incorporated into this database. TWBID Revision 2.1, Data Version 4.09 (Software Version 3.12) was used to develop the data for the *2003 Update Report*, while TWBID Revision 2.1, Data Version 4.16 (Software Version 3.13) was used for the *PABC-2004 Inventory Report*. A complete listing of the changes, as of March 18, 2005, associated with each Data Version (D0.00 through D4.16) of TWBID Revision 2.1 is presented in Appendix A of Leigh et al. 2005b.

Subsequent to the PABC-2004, management of the data on WIPP waste inventory was assigned to Los Alamos National Laboratory – Carlsbad Operations (LANL-CO). LANL-CO is responsible for data collection, data management and quality assurance (QA). The umbrella document for QA of the WIPP inventory is LCO-QPD-01 (LANL 2008a). Prior to 2006, WIPP waste inventories were prepared at irregular intervals. However, beginning in 2006, DOE started publishing waste inventories annually, and ATWIR 2007 (period ending December 31, 2006) was the first in the planned series of annual inventory reports. Revising the inventory on an annual basis tends to reduce database errors.

LANL-CO created the Comprehensive Inventory Database (CID) to collect, store and manage all inventory data for the WIPP team. The CID was created from the Transuranic Waste Baseline Inventory Database, Revision 2.1, Version 3.13, Data Version D.4.16 (subsequently referred to as TWBID Revision 2.1). TWBID Revision 2.1 was the database used for the PABC-2004/CRA-2009 PAs. During preparation of the December 31, 2006, inventory report (ATWIR 2007), inventory data from TWBID Revision 2.1 for each site were transferred to a Working Site Data Template (WSDT) that was sent to the respective waste generator sites for updating. The updated spreadsheets that were returned to LANL-CO from the waste generator sites provided the input for the CID.

To insure that the transfer of data from the TWBID Revision 2.1 to the WSDTs was complete and accurate, LANL-CO conducted the analysis described in McInroy (2006). The analysis involved manually checking the data entries for nine waste streams to insure that information had been correctly transferred from TWBID Revision 2.1 to the WSDT for the test waste stream. In addition, three calculations documenting data manipulation were checked via spreadsheets. These included Average Waste Parameter Density, Percent Containers Readily Shippable, and Projected Count for Current Form Container and Final Form Container. The analyses demonstrated that the required data were completely and accurately transferred from TWBID Revision 2.1 to the WSDTs.

Inventory information on emplaced wastes is collected in the WIPP Waste Information System (WWIS). This information must be transferred to the CID to insure that the CID inventory provides a complete picture of the disposal of all TRU wastes. To insure that data are accurately transferred and appropriate data transformations are correctly performed, LANL-CO developed the procedures described in INV-SAR-13 (Van Soest 2008) for the ATWIR 2008 inventory. This report describes, in detail, the database queries used to migrate the WWIS data into standardized CID Import Template files.

3.3   PERFORMANCE ASSESSMENT INVENTORY REQUIREMENTS

In 2008, DOE began producing a stand-alone, unscaled annual inventory report and a separate scaled PA-specific inventory report. Unlike ATWIR 2007, scaled inventory volumes were not reported in ATWIR 2008, nor were quantities of complexing agents, oxyanions, solidified cements and emplacement materials (ATWIR 2008, pg. 13). These types of information are needed for PA, and the data needs were filled by compilations included in PAIR 2008.

As described in Section 3.1 of PAIR 2008, the specific information needs for PA include the following:

- Waste stream volumes [in cubic meters (m^3)].

- Inventory of radionuclides on a waste stream basis for both contacted-handled (CH) and remote-handled (RH) TRU waste reported as activity in curies (Ci) and decayed to the years 2033, 2133, 2383, 3033, 7033, and 12033.
  - o   Disposal radionuclides: Am-241, Am-243, Cm-244, Cs-137, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Pu-244, Sr-90, Th-229, Th-230, Th-232, U-233, U-234, U-235, U-236, and U-238 on a waste stream basis.
  - o   Disposal radionuclides: Ac-227, Am-241, Am-243, C-14, Cf-249, Cf-251, Cf-252, Cm-243, Cm-244, Cm-245, Cm-246, Cm-247, Cm-248, Cm-250, Cs-135, Cs-137, I-129, Ni-59, Ni-63, Np-237, Pa-231, Pb-210, Pd-107, Pm-147, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Pu-244, Ra-226, Se-79, Sm-147, Sm-151, Sn-121m, Sn-126, Sr-90, Tc-99, Th-229, Th-230, Th-232, U-232, U-233, U-234, U-235, U-236, U-238, and Zr-93 on a WIPP scale basis.

- Inventory of all non-radiological components (WMPs) that are tracked on a waste stream basis for both CH and RH TRU waste.
  - o   The WMPs found in the waste include iron-based metal/alloy, aluminum-based metal/alloy, other metal/alloys, other inorganic materials, vitrified materials, CPR material, solidified inorganic material, solidified organic material, cements and soils. The non-radiological inventory for packaging includes steel, plastic/liners and lead from RH TRU waste. All WMPs and packaging materials are reported in average densities (kg/m^3).

- Inventory of any other non-radiological waste materials, not included in existing WMPs, that are discovered that account for a significant portion (greater than 5% by weight or volume) of a waste stream.

- Inventory of CPR and other biodegradable materials used to facilitate emplacement of waste and magnesium oxide (MgO) in WIPP, supplied as average densities (kg/m^3) for both CH and RH TRU waste.

- Inventory of organic complexing agents, oxyanions (sulfate, nitrate and phosphate), and cements reported in masses (kg).

- For emplaced waste, waste stream-level inventories of disposal radionuclides and non-radiological average densities for WMPs.

The WIPP waste inventory also includes large amounts of data not specifically required for PA, but that are used by DOE for other management purposes.

3.4 CHANGES FROM THE PABC-2004 INVENTORY TO ATWIR 2007 AND ATWIR 2008 INVENTORIES

The principal changes to the WIPP inventory since the publication of TBWIR 2004, which was used as the basis for the PABC-2004 and CRA-2009, are documented in ATWIR 2007 as follows (ATWIR 2007, Executive Summary, pg. 3):

- *Paducah's Gaseous Diffusion Plant TRU waste was re-categorized from WIPP- bound to potential, since a waste processing method has not been determined.*

- *Classified waste at all DOE TRU waste sites was categorized as potential TRU waste, since proper sanitization has not been completed.*

- *Hanford Richland (RL) has categorized some of its 618-10 and 618-11 buried waste as potential TRU waste.*

- *Hanford RL K-Basin knock-out pot sludge has been re-categorized as potential TRU waste.*

- *Hanford Office of River Protection (RP) tank waste has been re-categorized as potential TRU waste.*

- *The two INL sodium-bearing waste streams have been re-categorized as potential TRU waste.*

- *Some small quantity sites were removed from the TRU waste inventory because they have been de-inventoried of TRU waste.*

- *Rocky Flats Environmental Technology Site has emplaced all of its TRU waste in the WIPP.*

- *TRU waste emplaced between the 1999 opening of the WIPP and December 31, 2006 (the inventory data cut-off date), was addressed.*

Significant changes in the ATWIR 2008 inventory, as compared to the ATWIR 2007 inventory, are summarized by DOE as follows (ATWIR 2008, Executive Summary, pg. 14):

- *Paducah's Gaseous Diffusion Plant TRU waste was re-categorized from potential to WIPP-bound, since a waste processing method has been determined.*

- *TRU waste emplaced between the 1999 opening of the WIPP and December 31, 2007 (the inventory data cut-off date), is addressed in this report.*

- *General Electric-Vallecitos Nuclear Center (GE-VNC) received a DOE contract and a defense determination for the waste in its Hot Cell; however, the waste remains in potential waste because the site did not provide radionuclides and waste material parameters (LANL-CO 2008b).*

- *Two new sites were added to this inventory collection: Babcock and Wilcox (BL) (Parks Township waste) and the Nuclear Radiation Development Site (NRD). Both sites are listed as potential waste sites. NRD is pursuing a defense determination (LANL-CO 2008c and LANL-CO 2008d). BL needs a defense determination for the Parks Township waste.*

- *Hanford RL and the Material Fuel Complex (MFC) have waste streams that exceeded the curie limit allowed in the LWA of 23,000 Ci/m^3. These two waste streams were changed from WIPP-bound to potential waste streams.*

- *Oak Ridge re-aligned all waste stream identifiers to match the identifiers of the waste stream they intend to ship to WIPP.*

- *The volume of the TRU waste stored on site at West Valley was reduced because much of the waste managed as TRU has been characterized as low-level waste.*

3.5   COMPARISON OF THE PABC-2004/CRA-2009 INVENTORY WITH THE PABC 2009 INVENTORY

3.5.1   Waste Volumes

3.5.1.1   Scaling Factors

Since the volumes of stored, projected and emplaced waste destined for the WIPP are less than the authorized volumes of 168,485 m^3 for CH TRU waste and 7,079 m^3 for RH TRU waste, it is necessary to scale waste volumes to the repository regulatory limits for PA calculations. In developing the scaling factors, only projected waste volumes are adjusted. The scaling factor for CH TRU waste, SF_{CH}, is calculated as follows:

$$SF_{CH} = (168,485 - (V_s + V_e))V_p \,,$$

where V_s is the volume of stored waste, V_e is the volume of emplaced waste, and V_p is the volume of projected waste. The scaling factor for RH TRU waste is similarly calculated using the appropriate RH volumes and the volume limit of 7,079 m^3. Scaling factors based on the three most recent inventories are presented in Table 3-2.

Table 3-2.   WIPP Volume Scaling Factors

Waste	PABC-2004/CRA-2009	PAIR 2008/PABC-2009
CH TRU	1.48	5.72
RH TRU	0.861	4.87

Source: PAIR 2008, Table 5-1

At the time the PABC-2004/CRA-2009 inventory was developed, stored and projected RH TRU waste exceeded the authorized limit, resulting in a scaling factor of less than one. Since that time, a significant amount of waste at Hanford has been reclassified as potential waste and consequently removed from the active WIPP inventory. The scaling factor for CH TRU waste is also impacted by the decision to reclassify certain Hanford waste streams as potential waste.

3.5.1.2   CH TRU Waste Volumes

Table 3-3 compares the stored, projected and emplaced waste volumes by waste generator site for CH TRU, based on the PABC04, ATWIR 2007 and ATWIR 2008 inventories. The reported values are for unscaled volumes. The emplaced waste in the PABC04 was as of the September 30, 2002, data call. Ongoing waste disposal has increased the quantity of emplaced waste to 4.6E+04 at the end of 2006, and to 5.2E+04 at the end of 2007.

Table 3-3.   Comparison of Unscaled CH TRU Waste Volumes for PABC-2004/CRA-2009 and ATWIR 2008/PABC-2009 Inventories

Site	Stored CH TRU (m^3)	Projected CH TRU (m^3)	Emplaced CH TRU (m^3)	Stored CH TRU (m^3)	Projected CH TRU (m^3)	Emplaced CH TRU (m^3)
	PABC-2004/CRA-2009			ATWIR 2008		
Hanford	1.7E+04	5.5E+03	9.8E+01	2.0E+04	0.0E+00	3.3E+03
INL	6.1E+04	1.8E+04	2.9E+03	4.0E+04	0.0E+00	2.1E+04
LANL	1.2E+04	3.3E+03	2.7E+02	1.1E+04	8.5E+02	1.5E+03
ORNL	0.0E+00	4.5E+02	0.0E+00	6.9E+02	1.9E+02	0.0E+00
RFETS	5.4E+03	2.8E+03	4.3E+03	0.0E+00	0.0E+00	1.5E+04
SRS	1.3E+04	2.4E+03	2.0E+02	5.5E+03	4.5E+03	1.1E+04
SQS	1.2E+03	2.9E+03	0.0E+00	5.8E+02	1.1E+03	6.6E+02
Total	1.1E+05	3.5E+04	7.7E+03	7.8E+04	6.7E+03	5.2E+04

Sources: Leigh et al. 2005b, Tables 4 and 5; ATWIR 2008, Table 3-1.

3.5.1.3   RH TRU Waste Volumes

As shown in Table 3-4, anticipated waste volumes (sum of stored plus projected) for RH TRU decreased from 7.4×10^3 m^3 in the PABC-2004/CRA-2009 to 3.4×10^3 m^3 in the ATWIR 2007. This latter value is well below the established disposal limit of 7,079 m^3 for RH TRU waste.

Table 3-4. Comparison of Unscaled RH TRU Waste Volumes for PABC-2004/CRA-2009 and ATWIR 2008/PABC-2009

TRU Generator Site	Stored RH TRU (m^3)	Projected RH TRU (m^3)	Stored RH TRU (m^3)	Projected RH TRU (m^3)
	PABC-2004/CRA- 2009		ATWIR 2008	
Hanford	4.9×10^3	1.1×10^3	8.1×10^2	3.6×10^2
INL	2.2×10^2	0.0×10^0	2.9×10^2	0.0×10^0
LANL	1.3×10^2	0.0×10^0	9.8×10^1	0.0×10^0
ORNL	0.0×10^0	6.6×10^2	4.3×10^2	1.1×10^2
SRS	0.0×10^0	2.3×10^1	4.6×10^1	3.6×10^1
SQS	9.5×10^1	3.1×10^2	4.7×10^1	5.7×10^2
Totals	5.3×10^3	2.1×10^3	1.7×10^3	1.1×10^3

Sources: Leigh et al. 2005b, Table 6; ATWIR 2008, Table 3-2.

The principal reason for the decrease in RH TRU waste volumes was that tank wastes from the Hanford Office of River Protection were removed from the PABC-2004/CRA-2009 inventory and reclassified as potential wastes.

RH TRU waste shipments to the WIPP began in 2007, and by the end of the year, 88 m^3 of RH TRU from Idaho National Laboratory (INL) had been emplaced in the WIPP (ATWIR 2008, Table 3-2).

The sum of the anticipated and emplaced RH TRU waste volumes remains well below the established limit of 7,079 m^3.

3.5.2 Radionuclide Inventory

The containment requirements for the WIPP disposal system are defined in 40 CFR Part § 191.13, "Containment Requirements," which states in part that:

> *(b) Disposal systems for spent nuclear fuel or high-level or transuranic radioactive wastes shall be designed to provide a reasonable expectation, based upon PAs, that the cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system shall:*
> *(1) Have a likelihood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 (appendix A); and*
> *(2) Have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1 (appendix A).*

Table 1 of 40 CFR Part 191 Appendix A specifies the release limits for specific radionuclides. Footnote b of Table 1 specifies that the release limits are per "an amount of TRU waste containing one million Ci of alpha-emitting radionuclides with half-lives greater than 20 years." The normalized release R used in PA is defined as:

$$R= \sum(Q_i/L_i)(1 \times 10^6 \text{ Ci/C}) ,$$

where Q_i is the cumulative release of the *i*th radionuclide to the accessible environment over 10,000 years, L_i is the release limit for the *i*th radionuclide from Table 1 of Appendix A, and C is the total quantity of radioactivity in alpha-emitting TRU radionuclides with half-lives greater than 20 years. Thus for PA, it is necessary to quantify all of the radionuclides covered in Table 1 of Appendix A, and also to quantify TRU radionuclides with half-lives greater than 20 years.

For the PABC-2004/CRA-2009 PAs, C was 2.32×10^6 Ci (DOE 2009, Appendix PA, Section PA-2.2.1). This is based on the WIPP-scale inventory decayed to 2033, the assumed closure date for the repository. Similarly, based on the PAIR 2008 inventory, C is 2.61×10^6 Ci (PAIR 2008, Table A1). Of the 17 reported TRU radionuclides with half-lives greater than 20 years, Am-241, Pu-238, Pu-239, and Pu-240 contribute 99.99% of the total curies. The main difference in C between the PABC04 and the PAIR 2008 inventories is an increase of 3.45E+05 Ci in the Pu-238 content in the PAIR 2008 inventory.

Radioactive inventories for 2007, scaled to the full repository volume and decayed to 2033, are included in Table 3-5, based on PAIR 2008. These values are obtained by determining the activity density (Ci/m^3), based on the individual waste stream volume and activity content of each radionuclide, and scaling these values to the full repository volumes for RH TRU and CH TRU. The scaled activity densities are multiplied by the CH TRU repository limit of 168,485 m^3 and the RH TRU limit of 7,079 m^3, as appropriate to the waste stream categorization, to obtain the scaled quantities of radioactivity. For comparison, the PABC-2004 inventory reported on the same basis was 3.53E+06 Ci (Leigh and Trone 2005, Table 2). No significant changes in the quantity of radioactivity in the scaled inventory have occurred between the PABC-2004 inventory and the PAIR 2008 inventory.

Table 3-5.   Scaled Radioactivity in the WIPP Repository[a]

Waste Type	PABC-2004/CRA-2009		PAIR 2008/PABC 2009	
	Radioactivity (Ci)	Reference	Radioactivity (Ci)	Reference
CH TRU		--	3.10E+06	PAIR 2008, Table A.1
RH TRU	--	--	3.50E+05	PAIR 2008, Table A.1
Total	3.53E+06	Leigh et al. 2005b, Table 2	3.45E+06	--

a – Decayed to 2033

3.5.3   Non-Radioactive Waste Components

3.5.3.1   Materials Limits

According to 40 CFR § 194.24(c):

> *For each waste component identified and assessed pursuant to paragraph (b) of this section, the Department shall specify the limiting value (expressed as an upper or lower limit of mass, volume, curies, concentration, etc.), and the associated uncertainty (i.e., margin of error) for each limiting value, of the total inventory of such waste proposed for disposal in the disposal system.*

In accordance with this requirement, the DOE specified the following limiting values for waste material components: ferrous metals – minimum 2×10^7 kg; CPR maximum – 2×10^7 kg; free water emplaced with the waste – maximum 1,684 m^3; and nonferrous metals (metals not containing iron) – minimum 2×10^3 kg. These limits on waste material components have remained unchanged since the CCA was published (DOE 2009, 24.3.5[3]).

3.5.3.2   *Waste Material Parameters*

The WIPP waste inventory maintains the densities of the components comprising each waste stream and types of packaging materials used to emplace the waste streams. Complex-wide waste material densities are obtained by rolling up the waste material densities and waste stream volumes for each waste stream, based on data calls to the sites. The calculational methodology (described in Section 2.2.2.1 of ATWIR 2008) is summarized here for each type of waste material (WM_m). For the ith waste stream:

$$WM_{mi} = \rho_{i \times} v_i ,$$

where ρ_i is the density (kg/m^3) of the specific waste material (e.g., Fe-based metals) in the ith waste stream, and v_i is the volume of the ith waste stream (m^3). Both of these quantities are provided from the site data calls. WM_{mi} is the mass of the specific waste material in the ith waste stream, calculated from the data call information. This mass is then summed over all waste streams to determine the total mass (kg) of the specific waste material in the repository:

$$WM_M = \sum_i WM_{mi}$$

The final step involves dividing the total mass of the waste material (WM_M) by the total waste volume (V) of stored, projected and emplaced waste, to obtain the waste material density (WM_P) for all the identified WIPP-bound waste streams:

$$WM_P = WM_M /V$$

Minimum quantities of ferrous metals are specified in accordance with 40 CFR § 194.24(c). This material is necessary to control the redox potential of the repository brines, insuring that actinide elements are maintained in their lower, and therefore less soluble, oxidation states (DOE 2009, Appendix SOTERM, SOTERM-2.3.4). Data in the PAIR 2008 inventory show that the CH TRU packaging materials contain adequate ferrous metals to exceed the 2×10^7 kg minimum requirement for the repository (see Table 6-1).

A significant decrease in the amount of lead in packaging materials occurred between the PABC-2004 and the PABC-2009 inventories. This decrease is attributable to a changed assumption as to the material used to plug the RH TRU waste canisters. It was originally assumed that a lead plug would be used, but it was subsequently determined that a cement plug would provide sufficient shielding.

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[3] This notation refers to Section 24.3.5 under DOE's discussion of 40 CFR 193.24.

3.5.3.3   *Organic Ligands*

Organic ligands can form dissolved complexes with actinide elements in the waste, resulting in increased actinide solubilities. Consequently, ligands are tracked in the WIPP waste inventory. Masses of complexing agents for the PABC-2004 and PABC-2009 are compared in Table 3-6. Greater quantities of all species except sodium oxalate are present in the PABC-2009 inventory. At the time the PABC-2004 was developed, the presence of organic ligands was not predicted in any projected waste streams, so the results of the scaled and unscaled inventories were the same. However, the PAIR 2008 inventory included three waste streams containing organic ligands that also had projected waste volumes (LA-TA-55-19 – 143.1 m^3; LL-M001 – 255 m^3; LL-W018a – 234.2 m^3). The LANL waste stream (LA-TA-55-19) contains no ethylenediaminetetraacetic acid (EDTA), but does contain acetic, citric and oxalic acids. The Lawrence Livermore National Laboratory (LLNL) waste streams (LL-M001 and LL-W-018a) account for about 9% of the EDTA mass (assumed to be NaEDTA). Most of the EDTA mass from LLNL results from applying the CH TRU scaling factor of 5.72 (see Table 3-2) to the projected waste. These two LLNL waste streams combined have a scaled volume of 3,050 m^3 and contain a scaled mass of 30.7 kg EDTA (PAIR 2008, Table 4-6 and Appendix B.1). Of this total mass, 2.6 kg are associated with stored waste, 4.9 kg are associated with projected waste, and 23.2 kg are associated with the incremental volume calculated by scaling the projected waste to the repository volume limit. Thus, about 75% of the EDTA mass in these two waste streams results from scaling. As the inventory becomes better refined over time, it is likely that the quantity of organic ligands associated with scaled waste will decrease.

Table 3-6.   Disposal Mass of Complexing Agents

Compound	PABC-2004/CRA-2009[a] (kg)	PABC-2009[b] (kg)
Acetic Acid	1.42E+02	1.32E+04
Citric Acid	1.19E+03	5.68E+03
Oxalic Acid	1.38E+04	2.66E+04
Sodium Acetate	8.54E+03	9.70E+03
Sodium Citrate	4.00E+02	2.55E+03
Sodium EDTA	2.60E+01	3.54E+02
Sodium Oxalate	3.39E+04	6.46E+02

Sources: a – PAIR 2008, Table 5-7; b – PAIR 2008, Table 4-7

Complexing agents were reported in PAIR 2008 for the first time for 21 waste streams.

Details of how the CID was queried to obtain data on organic ligands for inclusion in PAIR 2008 are presented in Lott 2009. This QA document includes results of hand calculations demonstrating that the CID queries produced accurate results.

3.5.3.4   *Total Mass of CPR*

The total mass of CPR is summarized in Table 3-7. The total CPR mass has decreased 25% from that used in the PABC-2004/CRA-2009 to that used in PABC-2009 (based on ATWIR 2008/PAIR 2008).

Table 3-7.   Summary of CPR Masses in Recent WIPP Inventories

Material	PABC-2004/CRA-2009 (kg)	ATWIR 2008/PAIR 2008 (kg)
CH Waste		
Cellulosics	1.01E+07	6.74E+06
Rubber	2.19E+06	9.44E+05
Plastics	7.24E+06	6.40E+06
CH Packaging		
Cellulosics	0.00E+00	8.59E+05
Rubber	0.00E+00	0.00E+00
Plastics	2.86E+06	2.70E+06
RH Waste		
Cellulosics	6.58E+05	1.56E+05
Rubber	4.74E+05	4.67E+04
Plastics	5.66E+05	1.98E+05
RH Packaging		
Cellulosics	0.00E+00	0.00E+00
Rubber	0.00E+00	0.00E+00
Plastics	2.19E+04	9.91E+04
Emplacement Materials		
Cellulosics	2.07E+05	2.26E+05
Rubber	0.00E+00	0.00E+00
Plastics	1.48E+06	1.11E+06
TOTAL	2.43E+07	1.94E+07

3.6   VERIFICATION OF PARAMETERS USED IN PA

The use of all inventory-related parameters in the PA for CRA-2009 was reviewed as discussed in the 2010 CRA Parameters TSD (EPA 2010b). The review included confirmation that the new parameters related to emplacement materials had been included. All inventory-related parameters were correctly implemented in the CRA-2009 PA and the PABC-2009 PA.

3.7   OTHER REVIEW ACTIVITIES

EPA verified the radioactive decay calculations in ATWIR 2008 by conducting independent spot checks of the ORIGEN 2.2 calculations. These calculations demonstrated that the LANL/DOE results are appropriate for use in PA. EPA also spot-checked various randomly selected values in the tables appended to PAIR 2008 and determined that the selected values were correct. Selected values of EPA units in Table 1 of Fox et al. 2009 were also checked to insure that the EPA units were correctly calculated using the data from Table A1 of PAIR 2008.

A detailed review of the functionality of the various codes used to process inventory information is included in the Models and Codes TSD (EPA 2010c).

During the course of its review of the CRA-2009 and PABC-2009 documents, EPA raised completeness issues in several letters to DOE (Cotsworth 2009a and 2009b; Kelly 2009 and 2010), and DOE provided responses in a companion series of letters (Moody 2009a, 2009b and 2009c; Moody 2010a and 2010b). The issues and responses are summarized in some detail in

Appendix B of EPA 2010a. EPA is satisfied that DOE has adequately responded to the inventory-related completeness comments, and there are no unresolved questions.

3.8   CONCLUSIONS

The waste inventory used in the CRA-2009 PA was basically the same as used in the PABC-2004. The PABC-2004 inventory was thoroughly reviewed by EPA as part of the 2006 recertification decision, and findings were documented in the 194.24 CARD (EPA 2006a) and in the Inventory TSD (EPA 2006b). One minor change was to introduce six new parameters related to the densities of CPR used in emplacement materials. Although it was intended that emplacement materials should be included in the PABC-2004 PA, they were inadvertently omitted. This omission, which would have only a minor impact on PA results, was corrected in the CRA-2009 PA. Inclusion of the appropriate new parameters was verified in the CRA-2009 and PABC-2009 parameter reviews discussed in the Parameter TSD (EPA 2010b).

In 2006, DOE switched from an approach where inventories were developed on an ad hoc basis to one where the inventories were developed annually. The adoption of the annual approach reduces sources of error in the inventory. The waste inventory used in PABC-2009 was based on the ATWIR 2008/PAIR 2008 inventory. This was the second annual inventory. During the course of its review, EPA examined the QA procedures used to populate the CID from the database used for PABC-2009, update the CID annually, and transfer data from the WWIS to the CID. In addition, procedures used to verify chemical components in the waste and estimate the quantities in the waste were reviewed. Spot checks were made of various calculated values in the inventory documentation, and the checked values were determined to be correct. EPA also determined that DOE had adequately responded to CRA-2009/PABC-2009 completeness comments related to inventory. On the basis of its review, EPA concluded that DOE has appropriate QA procedures in place to accurately document the WIPP waste inventory on an annual basis. EPA further concluded that the ATWIR 2008/PAIR 2008 inventory is appropriate for use in PA calculations.

4.0   MODELS AND CODES

DOE must demonstrate on an ongoing basis that PA computer software is in compliance with regulations outlined in 40 CFR § 194.22 "Quality Assurance" and 40 CFR § 194.23 "Models and Computer Codes." Since the Agency's certification of the CCA, DOE has added computer hardware and upgraded the computer software. In order to maintain compliance with 40 CFR § 194.22(a)(2)(iv) and 40 CFR § 194.23, DOE is required to conduct testing on the computer codes to ensure that they still function properly with new hardware and software.

PA calculations were included in the 1996 CCA (DOE 1996b), and in the subsequent 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 containment criteria in the regulations and was approved for disposal of transuranic waste in May 1998. PA calculations were also an integral part of the CRA-2004 (DOE 2004b). During their review of the CRA-2004, EPA requested that an additional PA calculation, referred to as the CRA-2004 Performance Assessment Baseline Calculation (PABC-2004) (Leigh et al. 2005a), be conducted with modified assumptions and parameter values (Cotsworth 2005).

In 2005, DOE made revisions to eight of the computer codes, including LHS, POSTLHS, CUTTINGS, DRSPALL, PANEL, SUMMARIZE, PRECCDFGF and CCDFGF. The Agency's findings with respect to the qualification of these eight computer codes on the Compaq ES40 and ES45 are described in detail in EPA 2006e. After reviewing the information summarized in EPA 2006d, the Agency concluded that the most recent versions of these eight codes are approved for use in compliance calculations on the Compaq ES40 and ES45 using OpenVMS 7.3-1.

In 2006, the DOE procured four Compaq ES47 machines to add to the PA computing resources of two Compaq ES40 and two Compaq ES45 machines. In addition to the hardware upgrades, the operating system OpenVMS 7.3-1 was upgraded to OpenVMS 8.2. Because of these changes in the operating system and the addition of a new computing platform, DOE has conducted regression testing for each PA software code to ensure that each code continues to function correctly.

In addition to modifications to the computer codes since the PABC-2004 was issued, additional PA calculations were completed for and documented in the CRA-2009. The CRA-2009 PA included a number of technical changes and corrections, as well as updates to parameters and improvements to the PA computer codes (Clayton et al. 2008). The EPA requested that additional information, which was received between the commencement of the CRA-2009 PA modeling (December 2007) and the submittal of the CRA-2009 (March 2009), be included in an additional PA calculation (Cotsworth 2009a), referred to as the 2009 Compliance Recertification Application Performance Assessment Baseline Calculation (PABC-2009). The PABC-2009 analysis is guided by AP-145 (Clayton 2009a). Long (2010) documents the hardware, software, access control and run control systems, as well as the procedures used to perform the PABC-2009.

The Agency's findings with respect to the qualification of the versions of the codes used to support PABC-2009 and running on the Compaq ES40, ES45, and ES47 machines with

OpenVMS 8.2 are documented in EPA 2010c. The Agency concluded that the PABC-2009 versions of the computer codes running on the Compaq ES40, ES45, and ES47 machines with OpenVMS 8.2 are approved for use in WIPP PA compliance calculations.

5.0   PARAMETERS

Changes to the WIPP parameter database between the PABC-2004 (EPA 1998c) and the PABC-2009 occurred in two steps and were the subject of a two-stage Agency review. The first stage evaluated changes occurring between the PABC-2004 PA and the CRA-2009 PA, and the second stage evaluated changes occurring between the CRA-2009 PA and the PABC-2009 PA. Both stages of the Agency review are documented in EPA 2010b. These reviews assessed the transcription accuracy, documentation and traceability of changes to the parameter values and metadata that have occurred in the DOE's Performance Assessment Parameter Database (PAPDB) since the PABC-2004. A secondary objective was to determine if all parameters used in the PA calculations were in the PAPDB. The results of these reviews are summarized below.

No significant database problems were identified in the Agency's review. Of the approximately 1,700 parameters in the PAPDB, 255 changes were made since 2004 that included 109 new parameters and 146 changes to the values of existing parameters. Most of the new parameters were introduced to either support new chemistry models or were replacements for parameters that were previously hand-coded into the input files of the PA codes. The Agency recommended transferring parameters to the PAPDB because of the enhanced traceability that the database provides. Changes to the values of existing parameters occurred primarily because of an update to the waste inventory that prompted not only inventory changes, but also changes in solubility and density data. Other changes occurred due to updated hydrogeologic analyses and updated Delaware Basin drilling and plugging practices. All parameter distributions, values and units were correctly entered into the PAPDB, and were technically adequate and appropriate.

Representative samples of supporting documents listed in the PAPDB were checked for retrievability from the WIPP Records Center, maintained by SNL in Carlsbad, and DOE committed to correct a single concern that was identified. A database-code interface evaluation was performed for all new and changed parameters, and the correct parameter values were retrieved from the PAPDB for each parameter. Changes to the PA input file codes were reviewed for the presence of hand-coded parameter values that may have little traceability and would be better drawn from the PAPDB. Several parameters were moved into the PAPDB as a result of this review, and DOE committed to provide additional code comments to enhance traceability for those hand-coded values used as numerical and run controls not appropriate to be drawn from the PAPDB. Updated procedures for developing, documenting, controlling, and changing parameters and for entering those parameters into the PAPDB, were also reviewed. The Agency found all procedural changes to be consistent with earlier versions and found all revisions to be appropriate.

DOE committed to correct all database issues that were identified in these reviews and no Agency concerns related to the PABC-2009 database remain outstanding.

6.0   GAS GENERATION BY MICROBIAL DEGRADATION AND ANOXIC CORROSION

Anoxic corrosion is expected to affect WIPP repository performance by consuming water in brine, generating gas and maintaining reducing conditions in the repository. Microbial degradation of CPR may influence WIPP repository performance because of its effects on repository chemistry and gas generation. The Gas Generation conceptual model includes the assumption that radiolysis of water in the waste and brine and radiation of plastics and rubber in the waste will not have significant effects on the amounts of gas generated (SC&A 2008); EPA (2010e) reviewed this assumption and concluded that the available evidence indicates that radiolytic gas generation would be expected to have negligible effects on repository performance. As a result, only gas generation by anoxic corrosion and microbial degradation of CPR are expected to significantly affect repository performance.

6.1   ANOXIC CORROSION

Relatively large quantities of reduced iron will be present in the repository in the form of steel waste containers and as iron-based metals and alloys in the waste. The most recent inventory estimates of the densities of iron-based waste material and packaging materials in CH and RH waste are provided by Crawford et al. (2009, Tables 5-4 and 5-5). These densities, multiplied by the scaled volumes of CH and RH waste, indicate that over 51,000 metric tons of iron-based materials will be present in the repository at closure (Table 6-1).

Table 6-1.   Inventories of Iron-Based Metals and Alloys in Waste and Steel Packaging Materials

Parameter	Density (kg/m^3)	Disposal Volume (m^3)	Mass (kg)
CH Waste Iron-Based Metal and Alloys	81	168,485 m^3	13,647,285
CH Steel Packaging Materials	190	168,485 m^3	32,012,150
RH Waste Iron-Based Metal and Alloys	170	7,079 m^3	1,203,430
RH Steel Packaging Materials	630	7,079 m^3	4,459,770
Repository Total			51,322,635

Source: Crawford et al. 2009

The Gas Generation conceptual model includes a number of assumptions related to iron corrosion (Wilson et al. 1996a and 1996b, SC&A 2008):

- The small amounts of oxygen trapped in the repository immediately after closure will be consumed by oxic corrosion or aerobic microbial degradation, and these processes will not generate a significant amount of gas

- Anoxic corrosion can occur in the repository as soon as the shafts are sealed

- Anoxic corrosion of steel in the repository cannot occur unless brine is present and in contact with the steel, and the corrosion rate is assumed to be a function of both brine saturation and steel surface area

- Carbon dioxide (CO_2) generated by microbial degradation of CPR will not passivate steel, because CO_2 will be consumed by reaction with the MgO backfill

- Hydrogen sulfide (H_2S) might passivate steel by forming FeS(s) on the steel surfaces if H_2S is produced in sufficient quantities; however, reducing chemical conditions would continue to be maintained by the FeS(s)

It was determined during peer review of the Gas Generation conceptual model that the quantities of aluminum in the repository are too small to cause significant gas generation (Wilson et al. 1996a, 1996b, 1997a, 1997b). EPA (2010e) evaluated whether the quantities of metals other than iron, such as lead and aluminum, would be expected to significantly affect gas generation using the PABC09 inventory data. The quantities of iron in the WIPP repository at closure will be much greater than the quantities of other metals, based on the PABC09 inventory. EPA (2010e) concluded that the effects of relatively small amounts of gas production from anoxic corrosion of other metals will have insignificant effects on repository performance.

Anoxic corrosion of iron in the waste and waste containers produces hydrogen (H_2). The chemical reactions that represent the stoichiometry of anoxic corrosion of iron in the WIPP repository are:

$$Fe + (x+2) \, H_2O \leftrightarrow Fe(OH)_2 \bullet x H_2O(s) + H_2 \tag{1}$$
$$Fe + H_2S \leftrightarrow FeS(s) + H_2 \tag{2}$$

Gas generation by anoxic corrosion of iron is implemented in PA by assuming the humid corrosion rate is equal to zero, whereas the inundated corrosion rate is a sampled parameter uniformly distributed from zero to 3.17×10^{-14} m/sec (Fox 2008). The humid and inundated rate parameters were reviewed and approved by EPA (1998c) at the time of the CCA PAVT.

The anoxic corrosion rate parameters and implementation have not changed since the CCA PAVT was reviewed and approved by EPA (1998e). Since the CCA PAVT, reviews of the iron corrosion rate parameters and PA implementation have supported the conceptual model and approach used to model iron corrosion for WIPP PA (MFG 2000, TEA 2004). Consequently, the Gas Generation conceptual model assumptions related to iron corrosion and implementation of anoxic corrosion in the PABC09 remain adequate.

6.2 MICROBIAL GAS GENERATION

Cellulosics, plastics and rubber are present in WIPP waste and in waste emplacement and packaging materials. Microbial gas generation in the WIPP repository can occur because microbes are likely to be naturally present at the repository horizon or introduced with the waste. As these microbes utilize CPR materials as a carbon source, production of CO_2 could acidify repository brines or increase the solubility of actinides by carbonate complexation. To control chemical conditions and limit the possible effects of acidic conditions and carbonate complexation on actinide solubilities, MgO backfill is included in the repository to react with CO_2 and maintain mildly alkaline conditions with low CO_2 fugacity consistent with relatively low actinide solubilities.

6.2.1 Probability of Significant Microbial Degradation

DOE (1996b) assumed that microbial degradation of CPR could be limited by the long-term viability of microbes in the repository, and uncertainty associated with whether microbes would consume plastics and rubbers was also considered important in development of the conceptual model. Significant microbial gas production was assumed to occur in only half the realizations for the CCA PA, PAVT and CRA-2004 PA because of uncertainties associated with microbial processes. In half of the realizations in which significant microbial consumption of CPR occurred (one quarter of all realizations), only cellulosics were assumed to be consumed by microbial activity. In the remaining half of the realizations with significant microbial consumption of CPR (one quarter of all realizations), all CPR materials, including plastics and rubber, were assumed to be consumed by microbial activity (DOE 2004b, Section 6.4.3.3).

During the review of the CRA-2004, EPA (2006d) examined information regarding the probability of microbial degradation of CPR. EPA (2006d) concluded that the probability of significant microbial degradation of cellulosic materials should be higher than assumed for the CCA PA, PAVT and the CRA-2004 PA, and directed DOE to assume that microbial degradation of cellulosics would occur in all realizations (Cotsworth 2005). Because only limited degradation of rubber materials was observed and no degradation of plastics was observed, there was no evidence that the probabilities of plastics or rubber degradation assumed for the CCA PA and PAVT should be revised. For the PABC04, CRA-2009 PA and PABC09, significant microbial degradation of only cellulosics was assumed to occur in 75% of the realizations, and significant microbial degradation of cellulosics, plastics and rubber was assumed to occur in the remaining 25% of the realizations. EPA (2006c) found that these probabilities of significant microbial degradation of CPR were consistent with the available data and were an adequate response to EPA's request that significant microbial degradation should be assumed to occur in all PABC04 realizations. No additional data regarding the probabilities of microbial degradation of CPR have been identified since the PABC04. Consequently, the probabilities used in the PABC09 remain appropriate.

6.2.2 Microbial Degradation Reactions

The same conceptual model of microbial gas generation reactions in the WIPP repository was used for the CCA-PA, PAVT and CRA-2004 PA. It was assumed that microbial degradation of CPR may occur in the repository and produce methane [CH_4] and CO_2. The major pathways for microbial degradation of CPR are predicted to include the reactions:

$$C_6H_{10}O_5 + 4.8\ H^+ + 4.8\ NO_3^- \rightarrow 7.4\ H_2O + 6\ CO_2 + 2.4\ N_2 \tag{3}$$

$$C_6H_{10}O_5 + 6\ H^+ + 3\ SO_4^{2-} \rightarrow 5\ H_2O + 6\ CO_2 + 3\ H_2S \tag{4}$$

$$C_6H_{10}O_5 + H_2O \rightarrow 3\ CH_4 + 3\ CO_2 \tag{5}$$
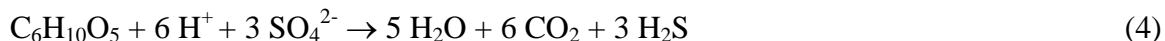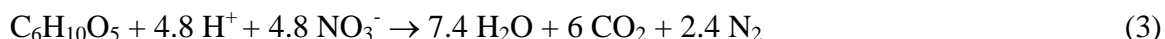
where $C_6H_{10}O_5$ is the chemical formula for cellulose monomer. In reactions (3) and (4), one mole of CO_2 is produced for each mole of organic carbon consumed. Reaction (5) produces only 0.5 moles of CO_2 per mole of organic carbon consumed. Reactions (3) to (5) are predicted to proceed sequentially according to the energy yield of the reactions (Wang and Brush 1996). As

the denitrification and sulfate-reduction reactions [reactions (3) and (4), respectively] proceed, DOE predicted that they would consume the limited amounts of nitrate [NO_3^-] and sulfate [SO_4^{2-}] in the WIPP waste inventory and produce limited quantities of nitrogen [N_2] and hydrogen sulfide [H_2S]. In both the CCA and the CRA-2004, DOE predicted that the methanogenesis reaction (5) would be the dominant reaction pathway and, consequently, that approximately half of the CPR carbon consumed would be converted to CO_2 (DOE 1996b, Appendix SOTERM, Section 8.2.2; DOE 2004b, Appendix PA, Attachment SOTERM, Section 2.2.2).

During a review of a Planned Change Request (PCR) to allow disposal of compressed waste in the WIPP repository, EPA reviewed information from DOE regarding the amounts of sulfate available for CPR degradation by sulfate reduction (reaction 4), and determined that DOE did not adequately account for sulfate in the brine and sulfate-bearing minerals in the Salado Formation (TEA 2004). EPA considered the available information and the uncertainty associated with possible microbial processes in the repository, and directed DOE to assume that all CPR carbon could be converted to CO_2, unless new and convincing evidence was provided that methanogenesis would occur in the WIPP repository (Cotsworth 2004b, Marcinowski 2004). For the PABC04, CRA-2009 PA and PABC09, it was assumed that all CPR degradation will take place through denitrification and sulfate reduction (reactions 3 and 4). Consequently, these PA calculations have included the assumption that one mole of CO_2 is produced for each mole of CPR carbon that is consumed by microbial degradation. Because no new data have been identified that would reduce the amounts of sulfate available to repository brines, this assumption was appropriate for the PABC09.

6.2.3 Microbial Gas Generation Rates

Microbial gas production is assumed to occur at rates that depend on the availability of brine. The ranges of microbial gas generation rates used for the CCA PA, the CCA PAVT and the CRA-2004 PA (Tables 6-2 and 6-3) were determined using initial results from inundated and humid condition microbial degradation experiments with cellulose (Francis and Gillow 1994; Wang and Brush 1996; DOE 2004b, Appendix PA, Attachment PAR). Gas-generation rates for plastics and rubber are assumed equal to the rate for cellulose. The larger average carbon content by weight for plastics is accounted for by multiplying the mass of plastics by a factor of 1.7 for calculation of the gas generation rate (Wang and Brush 1996).

Table 6-2. Inundated Microbial Gas Generation Rates (WAS_AREA:GRATMICI) Used in PA

(moles CO_2/kg cellulose/sec)

Performance Assessment	Minimum	Maximum	Reference
CCA/PAVT and CRA-2004 PA	3.17100×10^{-10}	9.51290×10^{-9}	DOE (1996b), DOE (2004b)
PABC04, CRA-2009 PA and PABC09	3.08269×10^{-11}	5.56921×10^{-10}	Nemer et al. (2005), Fox (2008)

Table 6-3.   Humid Microbial Gas Generation Rates (WAS_AREA:GRATMICH) Used in PA

(moles CO_2/kg cellulose/sec)

Performance Assessment	Minimum	Maximum	Reference
CCA/PAVT and CRA-2004 PA	0.00	1.26840×10^{-9}	DOE (1996b, DOE (2004b)
PABC04, CRA-2009 PA and PABC09	0.00	1.02717×10^{-9}	Nemer et al. (2005), Fox (2008)

Based on data that had become available since the CCA PA and PAVT, DOE used a two-step process to simulate microbial gas production rates in the WIPP repository for the PABC04, CRA-2009 PA and PABC09 (Nemer et al. 2005, DOE 2009). The initially rapid rates of microbial gas production were simulated by increasing the initial pressure in the BRAGFLO input file. This "precharging" of the repository gas pressure was combined with the use of lower gas generation rates determined from long-term experimental data (Tables 6-2 and 6-3). EPA (2006b) reviewed the derivation of the humid and inundated microbial gas generation rates and found that they were reasonable and adequately supported by the available experimental data.

Nemer and Stein (2005) described the implementation of the revised microbial gas generation rates in BRAGFLO for the PABC04. Because DOE believed the humid rate should be lower than the inundated rate, the sampled humid and inundated rates were compared within BRAGFLO. If the sampled humid rate exceeded the sampled inundated rate, the humid rate was set equal to the inundated rate. For the CRA-2009 PA and PABC09, DOE applied a conditional relationship, so that the sampled inundated rate was used as the maximum value for humid rate sampling (DOE 2009, Section 23.11.5; Kirchner 2008). The effects of this change on predicted repository performance are likely to be small, and EPA (2010e) determined that this change was acceptable for the PABC09.

Gas generation during the early stages of the repository was accounted for in BRAGFLO for the PABC04, CRA-2009 PA and PABC09 by assuming a fixed amount of gas was present in the repository at the beginning of the calculations (Nemer et al. 2005, Appendix B). The amount of gas in the repository was assumed to be equivalent to the amount of gas generated per gram of cellulose at the point where the relatively rapid short-term rate changed to the slower long-term rate in the experiments used to evaluate the maximum long-term inundated rate. This initial amount of gas pressure was calculated for the PABC04, CRA-2009 PA and PABC09 using the CRA-2004 CPR inventory. EPA (2010e) evaluated the amount of CPR carbon in the PABC09 inventory and found that it was virtually unchanged from the CRA-2004 CPR carbon inventory. Consequently, the initial repository gas pressure used in the PABC09 remains appropriate.

6.3   CONCLUSIONS REGARDING PABC09 GAS GENERATION

The conceptual model and implementation of gas generation from anoxic corrosion used for the PABC09 continue to be supported by the available data. The microbial gas generation rates used for the PABC09 are appropriate for modeling gas generation rates from degradation of cellulosic materials, but may overestimate gas generation rates from the degradation of plastics and rubber. DOE accounted for uncertainties regarding the rates of plastic and rubber degradation in the WIPP repository environment by assuming plastic and rubber degradation occurs in only 25% of

the realizations. Based on the available data, the approach for modeling microbial gas generation rates was appropriate for the PABC09.

7.0   DISSOLVED AND COLLOIDAL ACTINIDE SOURCE TERMS

Actinides in the WIPP waste inventory may be mobilized in brines, either in brine that flows into the repository from the DRZ in the Salado Formation or brine that flows up a borehole that intersects both the repository and a pressurized brine region in the underlying Castile Formation. Actinides can be mobilized from the WIPP waste inventory in both dissolved and colloidal forms.

The actinides considered in the PA calculations include americium, curium, neptunium, plutonium, thorium and uranium. As part of the Chemical Conditions conceptual model, equilibrium is not assumed for redox reactions among the actinides. The actinide oxidation states predicted to persist in the WIPP repository environment over the long term are (DOE 1996b, Appendix SOTERM):

- Americium(III), curium(III) and thorium(IV)
- Plutonium(III) and plutonium(IV)
- Neptunium(IV) and neptunium(V)
- Uranium(IV) and uranium(VI)

The assumptions regarding the oxidation states were peer reviewed and approved for the CCA as part of the Dissolved Actinide Source Term and Chemical Conditions conceptual models (Wilson et al. 1996a, 1996b, 1997a, 1997b). These actinide oxidation state assumptions have been used for all WIPP PAs. Because it is assumed for PA that plutonium, neptunium and uranium may be present in either of two oxidation states, an oxidation-state parameter is sampled from a uniform distribution (DOE 2009, Appendix SOTERM-5.2; Fox 2008). For half of the PA realizations, the plutonium(III), neptunium(IV) and uranium(IV) oxidation states are assumed to be present, and for the other half of the PA realizations, the plutonium(IV), neptunium(V) and uranium(VI) oxidation states are assumed present. Americium and curium are assumed to be present in the +III oxidation state and thorium in the +IV oxidation state for all PA calculations. EPA (2010e) reviewed the actinide oxidation state information developed since the CCA PAVT and concluded that these oxidation state assumptions remained valid for the PABC09.

7.1   DISSOLVED ACTINIDE SOURCE TERM

Actinide solubilities are calculated for WIPP PA using thermodynamic modeling that depends on a number of assumptions related to chemical conditions in the repository and to the chemical behavior of the actinides in solution. Consequently, both the Chemical Conditions and Dissolved Actinide Source Term conceptual models are important for the calculation of dissolved actinide concentrations used in PA. These conceptual models are described in detail by SC&A (2008, Appendix A).

The Chemical Conditions conceptual model includes assumptions related to the mineralogy of the Salado Formation in contact with WIPP brines, the compositions of the Salado and Castile brines that may enter the repository and contact waste, organic ligand concentrations, and the reactions that may control important chemical parameters, including pH, redox and CO_2 fugacities. The Dissolved Actinide Source Term conceptual model includes assumptions about the oxidation states of the actinides, equilibrium of the brine with respect to precipitation-

dissolution reactions, the existence of reducing conditions in the repository, the important inorganic and organic constituents for determining actinide speciation in brines, and use of the Pitzer activity coefficient model.

7.1.1   FMT Code and Database

The FMT code is used to calculate the solubilities of the +III, +IV and +V actinides for WIPP PA. Because DOE has not developed an aqueous speciation and solubility model for the +VI actinides, uranium(VI) concentrations are assumed equal to a fixed value (Section 7.1.5). FMT calculations are performed using the Pitzer activity coefficient model. The CCA PA actinide solubility calculations were performed with FMT Version 2.0, and the CCA PAVT calculations were performed using FMT Version 2.2. FMT Version 2.4 was used for the CRA-2004 PA, PABC04, CRA-2009 PA and PABC09 actinide solubility calculations (Brush and Xiong 2003a; Brush and Xiong 2005a, Brush et al. 2009).

The FMT database has been revised several times since the CCA PAVT (Table 7-1). The database underwent significant revisions prior to the CRA-2004 PA actinide solubility calculations (Giambalvo 2002a, 2002b, 2002c, 2002d, 2002e, 2003). These changes included incorporation of aqueous speciation data for actinide-organic ligand complexes using data from Choppin et al. (2001), as well as other revisions. These revisions were reviewed and approved by EPA (2006c). Additional revisions were made to the FMT database before the PABC04. These changes included a revised standard chemical potential (μ^0/RT) value for the $Th(OH)_4^0$ aqueous species, correction of the molecular weight of oxalate and addition of data for a calcium-oxalate solid phase [whewellite, $CaC_2O_4 \cdot H_2O(s)$]. These changes were reviewed and accepted by EPA (2006d).

Table 7-1.   FMT Database Versions Used for WIPP PAs

Performance Assessment	FMT Database Version
CCA/PAVT	FMT_970407.CHEMDAT
CRA-2004	FMT_021120.CHEMDAT
PABC04, CRA-2009 PA and PABC09	FMT_050405.CHEMDAT

The FMT database used for the CRA-2009 and PABC09 actinide solubility calculations was the same version used for the PABC04 (Brush et al. 2009, Moody 2009a). DOE is required to update each compliance recertification application using all additional geologic, geophysical, geochemical, hydrologic and meteorological data that have become available since the previous compliance recertification application [40 CFR § 194.15(a)]. DOE (2009) qualitatively addressed recently available actinide solubility and aqueous speciation data, but did not revise the FMT database based on these data. Review of the information provided by DOE and other literature data by EPA (2010e) indicated that the FMT database was adequate for calculating actinide solubilities used in the PABC09. However, EPA (2010e) recommended that DOE perform a review and update of the FMT database prior to the CRA-2014 using available literature data.

7.1.2 Organic Ligands

Acetate, citrate, EDTA and oxalate are organic ligands that could potentially affect actinide solubilities, because these ligands are water soluble and present in significant quantities in the WIPP inventory (DOE 1996a). Possible concentrations of these ligands were estimated by DOE (1996b) for the CCA PA and PAVT using the inventory amounts and a brine volume of 29,841 m^3, which was the smallest quantity of brine in the repository that will support transport away from the repository (Larson 1996). The organic ligand concentrations calculated by DOE (1996b) are listed in Table 7-2. DOE (1996b, Appendix SOTERM, Section 5) determined that actinide solubilities would not be significantly affected by the presence of organic ligands because other constituents, including transition metals in the waste and magnesium from the MgO backfill, would compete with the actinides for binding sites on the organic ligands. EPA (1998d) reviewed the available data and concurred with DOE's assessment that organic ligands would not significantly affect actinide solubilities.

Table 7-2.   Ligand Concentrations Calculated for the CCA PAVT, PABC04 and PABC09

Ligand	CCA PAVT (m) (DOE 1996b)	PABC04 (M) (Brush 2005)	PABC09 (M) (Brush and Xiong 2009)
Brine Volume (m^3)	29,841	10,011	17,400
Acetate[a]	1.1×10^{-3}	1.06×10^{-2}	1.94×10^{-2}
Citrate[b]	7.4×10^{-3}	8.06×10^{-4}	2.38×10^{-3}
EDTA[c]	4.2×10^{-6}	8.14×10^{-6}	6.47×10^{-5}
Oxalate[d]	4.7×10^{-4}	4.55×10^{-2}	1.73×10^{-2}

a – Sum of acetic acid (CH_3COOH) and sodium acetate ($NaCH_3COO$)
b – Sum of citric acid ($C_6H_8O_7$) and sodium citrate ($NaC_6H_7O_7$)
c – Assumed monosodium EDTA
d – Sum of oxalic acid ($H_2C_2O_4$) and sodium oxalate ($NaHC_2O_4$)

Reported inventories for acetate, citrate, EDTA and oxalate changed between the CCA and the CRA-2004, including increased concentrations of acetate, changes in oxalate and citrate inventories that appear to have been caused by transposing the data during the CCA, and a decrease in the estimated inventory of EDTA (DOE 2004b, Appendix PA, Attachment SOTERM, Table SOTERM-4). DOE (2004b, Appendix PA, Attachment SOTERM, Sections 3.5 and 5.0) included the effects of acetate, citrate, EDTA and oxalate on the calculated solubilities of the +III, +IV and +V actinides used in the CRA-2004 PA. Brush and Xiong (2003c) calculated the organic ligand concentrations used in the actinide solubility calculations by dividing the total reported ligand inventory by 29,841 m^3 of brine (the minimum volume to support transport away from the repository) (Larson 1996; DOE 1996b). After the solubility calculations had been completed for the CRA-2004 PA, it was discovered that the organic ligand inventories were slightly in error (DOE 2004b; Brush and Xiong 2003b). However, because the corrected organic ligand inventories and concentrations were smaller than those used in the CRA-2004 PA solubility calculations, it was determined that using the incorrect organic ligand concentrations would conservatively overestimate actinide solubilities (DOE 2004b). EPA (2006d) reviewed the results of these calculations, as well as additional solubility calculations performed by Brush and Xiong (2004), to assess the sensitivity of the calculated actinide solubilities to varying concentrations of the organic ligands acetate, citrate, EDTA, lactate and oxalate. EPA (2006d) found that the solubilities of the +III actinides appear to be sensitive to the

assumed concentration of EDTA, but not to acetate, citrate, lactate or oxalate at the evaluated concentrations. The results of the FMT calculations indicated that varying concentrations of organic ligands did not change the predicted +IV actinide concentrations. The +V actinide solubilities appear to be strongly affected by organic ligand complexation because of complexation of +V actinides by oxalate and acetate. Review of the available information regarding complexation of uranium(VI) by organic ligands under anticipated WIPP repository conditions, including low-ionic-strength calculations performed by Wall and Wall (2004), indicated that organic ligand complexation would not significantly increase uranium(VI) solubilities because of the formation of relatively stable uranium(VI)-carbonate species.

For the PABC04 actinide solubility calculations, corrected masses of organic ligands reported by Crawford and Leigh (2003) were used to calculate ligand concentrations (Brush and Xiong 2005b). These masses were converted to moles and divided by a revised minimum brine volume of 10,011 m^3 (Stein 2005) to yield the organic ligand concentrations used in the actinide solubility calculations. The resulting organic ligand concentrations used for the PABC04 solubility calculations are compared to the PAVT organic ligands concentrations in Table 7-2.

The actinide solubilities used in the CRA-2009 PA were the concentrations calculated for the PABC04, so the most recent inventory data for organic ligands were not accounted for in the actinide solubility calculations. Inventory data reported by Crawford et al. (2009) showed that organic ligand quantities increased for acetic acid, citric acid, sodium citrate and sodium EDTA since the PABC04. Because of the potential effects of organic ligands on actinide solubilities, EPA instructed DOE to include the revised inventory of organic ligands in the PABC09 actinide solubility calculations.

DOE used the most recent inventory data (Crawford et al. 2009) and the most recent estimate of the minimum brine volume necessary for DBR (Clayton 2008) to calculate organic ligand concentrations for the PABC09 (Table 7-2, Brush and Xiong 2009). Because the most recent inventory data for organic ligands were incorporated in the actinide solubility calculations, the effects of the updated inventory on the dissolved actinide source term were accounted for in the PABC09 calculations. The aqueous speciation and solubility calculations were carried out both with and without the predicted organic ligand concentrations. The results obtained with organic ligands were used to determine dissolved actinide source term concentrations for the PABC09. Results of the calculations without organic ligands provide an indication of the effects of organic ligands on actinide solubilities in WIPP brines, and are also useful for comparisons to literature solubility and speciation data obtained without organic ligands.

7.1.3 Salado Formation and Castile Formation Brines

Small quantities of intergranular and intragranular Salado brines are associated with the bedded salt at the repository horizon. These brines are highly concentrated (ionic strengths up to 8 molar), with a composition of mostly sodium, magnesium, potassium, chloride and sulfate, and with smaller amounts of calcium, carbonate and borate. Two formulations of Salado brines have been used in WIPP laboratory experiments and PA calculations—Brine A and Generic Weep Brine (GWB) (Snider 2003). For the CCA PAVT, the Brine A formulation was used to simulate intergranular Salado brines. However, after the CCA PAVT, DOE determined that the GWB formulation more accurately represented the Salado intergranular brine composition. A detailed

discussion of GWB brine and a comparison of this brine to Brine A were provided by Snider (2003). DOE used the GWB formulation for the CRA-2004 PA actinide solubility calculations. EPA (2006d) reviewed DOE's use of the GWB brine formulation to model actinide solubilities for the CRA-2004 PA, and concluded that use of the GWB formulation in place of Brine A for the CRA-2004 PA and future actinide solubility calculations is appropriate. DOE has used the GWB formulation for all subsequent actinide solubility calculations, including the PABC09.

Castile brine may enter the repository if a borehole that penetrates the repository also penetrates an area of pressurized brine in the underlying Castile Formation. Borehole ERDA-6 encountered pressurized brine in the Castile Formation and EPA has determined that the composition of this brine is appropriate for use in WIPP PA. The ERDA-6 brine composition has been used to represent the likely composition of Castile brine in laboratory experiments and all WIPP PA calculations, including the PABC09.

7.1.4 Actinide Solubility Uncertainties

The actinide solubilities used in WIPP PA are constants; uncertainties in these values are accounted for in PA by sampling a cumulative distribution function representing uncertainty and multiplying the solubilities by the antilog of the sampled value to determine the actinide concentrations used in PA for each realization. The determination of the actinide solubility uncertainty distribution used in the CCA PA and PAVT was reviewed in detail by EPA (1998d). To obtain this distribution, DOE compared experimentally measured solubility data used to develop the solubility models in FMT to the concentrations predicted by curve-fitting with the code NONLIN (Babb 1996). DOE also compared solubilities reported in the literature with concentrations predicted using FMT for the conditions of the experiments. The population of differences from these comparisons was accumulated and used to generate a cumulative distribution. DOE excluded data for the +IV and +VI actinides from the evaluation, because these datasets were believed to be inconsistent or technically deficient. The remaining data consisted of +III actinide solubility measurements (139 values) and +V actinide solubility measurements (11 values). These data were combined to generate a single distribution, which ranged on a log scale from -2.0 to 1.4, with a mean value of 0.24 (Table 7-3). This distribution was used to represent the uncertainties associated with the solubilities for all four actinide oxidation states for the CCA PAVT and the CRA-2004 PA.

Table 7-3. **Comparison of the Thorium(IV) and Americium(III) Solubility Uncertainty Distribution Statistics for the CCA PAVT, PABC04 and the PABC09**

(Bynum 1996, Xiong et al. 2009)

Actinide Oxidation State	Thorium(IV)			Americium(III)		
Performance Assessment	CCA PAVT	PABC04	PABC09[a]	CCA PAVT	PABC04	PABC09[b]
Mean	0.24	0.108	-0.346	0.24	0.035	-0.142
Median	-0.09	0.075	-0.520	-0.09	-0.031	0.072
Standard Deviation	not reported	0.837	0.995	not reported	0.900	1.17
Maximum	1.4	2.40	3.30	1.4	2.85	2.70
Minimum	-2.0	-1.80	-2.25	-2.0	-3.00	-4.20

a – The PABC09 thorium(IV) statistics listed in Xiong et al. (2009) differed slightly from the summary statistics in the spreadsheet (PABC09 Th(IV) Uncertainty Analysis 091124.xls) provided to EPA: mean = -0.349, median = -0.517, standard deviation = 0.992, maximum = 3.19 and minimum = -2.21.

b – The PABC09 americium(III) statistics listed in Xiong et al. (2009) differed slightly from the summary statistics in the spreadsheet (PABC09 Am(III) Uncertainty Analysis 091124.xls) provided to EPA: mean = -0.145, median = 0.090, standard deviation = 1.17, maximum = 2.68 and minimum = -4.16.

Because the available solubility data and the FMT database had changed since the CCA PA and PAVT, EPA requested that DOE re-evaluate the uncertainties associated with the actinide solubilities for the PABC04, using the currently available actinide solubility data (Cotsworth 2004a, Comment C-23-16). DOE re-evaluated the uncertainties associated with actinide solubilities (Triay 2005, Xiong et al. 2004, Xiong et al. 2005). Separate evaluations of the solubility uncertainty distribution were carried out for the +III, +IV and +V actinide oxidation states. For each data point, the predicted solubility was calculated for the relevant experimental conditions using FMT. The difference value (D) was calculated using the predicted solubility (S_p) and measured solubility (S_m):

$$D = \log(S_m) - \log(S_p) \tag{6}$$

The difference values were used to develop histograms and cumulative distribution functions for the +III, +IV and +V actinide oxidation states. The difference values for all three oxidation states were also combined into a single distribution. The +III and +IV actinide solubility uncertainty distributions were sampled for the PABC04, but the +V actinide solubility uncertainty was not used. Neptunium is the only actinide expected to be present in the +V oxidation state in the equilibrium WIPP repository, and its inventory is insufficient to affect the long-term performance of the repository, regardless of its solubility (Brush et al. 2005, EPA 2006d).

A cumulative distribution function for the uranium(VI) solubility uncertainty was not created, because DOE has not developed a solubility model for the +VI actinides. DOE proposed to use the combined uncertainty distribution calculated with the +III, +IV and +V solubility data in combination with the estimated uranium(VI) concentration from Hobart and Moore (1996) for PA (Brush et al. 2005). EPA (2006d) determined that a single value representing the upper end of the solubility range for uranium(VI) that could be anticipated under repository conditions would be more defensible for use in the PABC04 (Section 7.1.5). EPA (2006d) reviewed the revised uncertainty ranges and found them to be adequate. DOE consequently used the revised

uncertainty distributions to represent the +III and +IV solubility uncertainties for the PABC04 and CRA-2009 PA.

During EPA's completeness review of the CRA-2009 (DOE 2009), EPA noted that additional data related to the solubilities of actinides had become available since the PABC04 (Cotsworth 2009a, Comment 1-23-3). EPA requested that DOE evaluate the possible effects of these additional data on the solubility uncertainty distributions. DOE prepared updated uncertainty distributions for the +III and +IV actinides that were sampled for the PABC09 (Xiong et al. 2009). EPA (2010e) reviewed these actinide solubility uncertainty distributions and found that DOE had in some cases inconsistently applied their stated criteria for selecting data used in the evaluation. However, EPA (2010e) determined that these inconsistencies had little effect on the mean releases calculated for the PABC09 and did not significantly affect the predicted repository releases. Consequently, EPA (2010e) found that the actinide solubility uncertainty distributions sampled for the PABC09 were adequate.

7.1.5   Dissolved Actinide Concentrations Used in PA

The FMT database includes actinide solubility and aqueous speciation data only for americium(III), thorium(IV) and neptunium(V). DOE uses the oxidation state analogy to extend the calculated americium(III), thorium(IV) and neptunium(V) solubilities to the other actinides and oxidation states important to WIPP PA. The oxidation-state analogy, part of the Dissolved Actinide Source Term conceptual model, is the assumption that all actinides in the same oxidation state will form the same aqueous species and isostructural compounds. Consequently, plutonium(III) and curium(III) solubilities in WIPP brines are assumed to be equal to calculated americium(III) solubilities, and uranium(IV), plutonium(IV) and neptunium(IV) solubilities are assumed to be equal to calculated thorium(IV) solubilities. Calculated neptunium(V) solubilities are used only for neptunium, because it is the only actinide predicted to be present in WIPP brines in the +V oxidation state.

Because DOE could not develop an adequate thermodynamic model for uranium(VI), fixed concentrations of 8.7×10^{-6} M (Salado brine) and 8.8×10^{-6} M (Castile brine) were used for the CCA PA and CCA PAVT. EPA (1998d) accepted the use of these uranium(VI) concentrations for the CCA PAVT because they were consistent with the available data, and uncertainties associated with these concentrations were adequately accounted for by the sampled uncertainty distribution (Table 7-3). These uranium(VI) concentrations and uncertainty distribution were also used for the CRA-2004 PA. EPA (2006d) carried out a review of the available uranium(VI) solubility data in NaCl brines and determined that a reasonable upper limit for uranium(VI) solubility in WIPP brines would be 10^{-3} M. EPA directed DOE to use the revised, higher uranium(VI) of 10^{-3} M for the PABC04 (Cotsworth 2005). Because this value was an upper limit, an uncertainty value was not sampled for uranium(VI) in the PABC04 calculations. This upper-limit concentration for uranium(VI) was also used for the PABC09. EPA (2010e) reviewed the available data regarding uranium(VI) solubilities in brine and concluded that this approach continued to be appropriate for the PABC09.

The effects of organic ligands were not included in the actinide solubility calculations for the CCA PAVT. At that time, the FMT database did not include aqueous speciation data for the

complexation of actinides by organic ligands. The potential effects of organic ligands were expected to be negligible because of competition for organic ligand binding sites by transition metals and magnesium (Section 7.1.2). For the CRA-2004 PA, PABC04, CRA-2009 PA and PABC09, the effects of organic ligands on actinide solubilities were included in the FMT calculations.

For all actinide solubility calculations performed for WIPP PA, it was assumed that actinide solubilities in brine mixtures would be adequately represented by calculations with the end-member brines. For the CCA PAVT, PABC04 and PABC09 actinide solubility calculations, it was assumed that the brines would be in equilibrium with the Salado minerals anhydrite and halite, as well as brucite $[Mg(OH)_2(cr)]$ and korshunovskite $[Mg_2Cl(OH)_3 \bullet 4H_2O(cr)]$[4] that would form from hydration of the MgO backfill. The mineral glauberite $[Na_2Ca(SO_4)_2]$ was allowed to precipitate from the brines in all calculations. In the PABC04 and PABC09 calculations that included organic ligands, the mineral whewellite also precipitated.

Magnesium oxide (MgO) backfill placed in the WIPP repository hydrates to form brucite. Brucite dissolution is expected to maintain mildly alkaline pH conditions in repository brines. Reaction of brucite with carbon dioxide $[CO_2]$ will control CO_2 fugacity and limit actinide solubilities in WIPP brines. The most stable magnesium-carbonate phase under repository conditions is magnesite $[MgCO_3(cr)]$. Because of the high energy of hydrolysis of the magnesium ion, magnesite does not precipitate directly from low-temperature solutions. Instead, metastable formation of hydrated magnesium carbonate phases, such as hydromagnesite $[Mg_5(CO_3)_4(OH)_2 \bullet 4H_2O(s)]$ and nesquehonite $[MgCO_3 \bullet 3H_2O(s)]$, are more likely to occur. Formation and metastable persistence of these hydrated magnesium carbonate phases result in higher CO_2 fugacities and higher predicted actinide solubilities. Because hydromagnesite and nesquehonite are not thermodynamically stable under repository conditions, they are expected to eventually dehydrate to form magnesite. After review of the available data, EPA (1997a, 1997b, 1998a, 1998d) determined that nesquehonite, if it formed in the repository, would rapidly convert to hydromagnesite. The rate of conversion of hydromagnesite to magnesite was predicted to be much slower. EPA (1998d) determined that the CCA PAVT actinide solubility calculations should include the assumption that reaction of brucite to form metastable hydromagnesite would control CO_2 fugacities in the WIPP repository, rather than the brucite-magnesite reaction. The assumption that the reaction of brucite to form hydromagnesite controls CO_2 fugacities in WIPP brines has been included in all subsequent actinide solubility calculations for WIPP PA. EPA (2010e) reviewed the available data and concluded that the MgO backfill will continue to control CO_2 fugacities under inundated conditions and maintain chemical conditions in WIPP brines that limit actinide solubilities. The current emplacement plan, MgO characterization data and reactivity testing procedure ensure adequate amounts of MgO are emplaced in each room. EPA (2010e) concurred with the use of the brucite-hydromagnesite reaction to control CO_2 fugacities for the PABC09 actinide solubility calculations.

The results of the actinide solubility calculations performed for the PABC09 are summarized in Table 7-4. The results obtained with organic ligands were used in the PABC09, and the results without organic ligands were provided to demonstrate the possible effects of organic ligands on actinide solubilities and allow for comparisons with literature data that do not include the effects

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[4] DOE has referred to this material as "phase 3."

of organic ligands. The presence of organic ligands affected the total predicted +III actinide solubilities, increasing the predicted americium(III) solubility in both GWB and ERDA-6 brine. Examination of the reported aqueous speciation of the +III actinides indicated americium(III)-EDTA complexation caused the higher predicted +III actinide solubilities (Table 7-5). The presence of organic ligands had essentially no effect on predicted +IV actinide solubilities in GWB or ERDA-6 brine (Table 7-4). The principal thorium aqueous species were predicted to be $Th(OH)_4^0$ and $Th(OH)_3CO_3^-$ both with and without organic ligands (Table 7-5). Organic ligands increased the predicted +V actinide solubility by approximately a factor of two (Table 7-4). Enhanced solubility of neptunium(V) in the presence of organic ligands was caused by the complexation of NpO_2^+ by acetate and oxalate (Table 7-5).

EPA (2010e) reviewed and approved the actinide solubility calculations carried out for the PABC09. For each PA realization, the actinide solubilities were used with a sampled parameter indicating whether relatively reduced [plutonium(III), uranium(IV) and neptunium(IV)] or oxidized [plutonium(IV), uranium(VI) and neptunium(V)] oxidation states would be present and with sampled uncertainty parameters for the solubilities of the +III and +IV actinides to calculate the actinide solubilities for each realization. In all realizations that had the higher assumed actinide oxidation states, the concentrations of neptunium(V) and uranium(VI) were constant values.

Table 7-4.   PABC09 Actinide Solubility Modeling Results with and without Organic Ligands

Brine	GWB		ERDA-6	
	With Ligands[a]	Without Ligands	With Ligands[a]	Without Ligands
pH (standard units)	8.69	8.69	8.98	9.02
pcH	9.40	9.40	9.68	9.73
Ionic Strength	7.64	7.59	6.77	6.72
Carbon dioxide fugacity (atm)	3.135×10^{-6}	3.135×10^{-6}	3.135×10^{-6}	3.135×10^{-6}
Sodium (M)	4.308	4.331	5.284	5.325
Potassium (M)	0.5209	0.5208	0.09607	0.09615
Magnesium (M)	0.5842	0.5590	0.1362	0.1060
Calcium (M)	9.798×10^{-3}	0.01039	0.01123	0.01129
Chloride (M)	5.399	5.440	5.232	5.255
Sulfate (M)	0.2097	0.1922	0.1760	0.1679
Total Carbon (M)	3.499×10^{-4}	3.502×10^{-4}	4.476×10^{-4}	4.709×10^{-4}
Boron (M)	0.1762	0.1762	0.06240	0.06245
Bromine	0.02967	0.02966	0.01089	0.01090
Oxalate (M)	1.246×10^{-3}	0.00	2.438×10^{-4}	0.00
Acetate (M)	0.02164	0.00	0.01921	0.00
EDTA (M)	7.217×10^{-5}	0.00	6.408×10^{-5}	0.00
Citrate (M)	2.655×10^{-3}	0.00	2.357×10^{-3}	0.00
Americium(III) (M)	1.656×10^{-6}	2.252×10^{-7}	1.514×10^{-6}	8.667×10^{-8}
Thorium(IV) (M)	5.626×10^{-8}	5.642×10^{-8}	6.982×10^{-8}	7.196×10^{-8}
Neptunium(V) (M)	3.905×10^{-7}	2.209×10^{-7}	8.746×10^{-7}	5.379×10^{-7}
Uranium(VI) (M)[b]	0.001	0.001	0.001	0.001
Solid Phases	Anhydrite, halite, brucite, korshunovskite, ThO_2(am), $KNpO_2CO_3$(s), $Am(OH)_3$(s), hydromagnesite, whewellite	Anhydrite, halite, brucite, korshunovskite, ThO_2(am), $KNpO_2CO_3$(s), $Am(OH)_3$(s), hydromagnesite	Anhydrite, halite, brucite, ThO_2(am), $KNpO_2CO_3$(s), $Am(OH)_3$(s), hydromagnesite, whewellite, glauberite	Anhydrite, halite, brucite, ThO_2(am), $KNpO_2CO_3$(s), $Am(OH)_3$(s), hydromagnesite
Output File Name	FMT_PABC09_GWB_HMAG_ORGS_005.OUT	FMT_PABC09_GWB_HMAG_NOORGS_006.OUT	FMT_PABC09_E6_HMAG_ORGS_013.OUT	FMT_PABC09_E6_HMAG_NOORGS_014.OUT

a – Results used for CRA-2009 dissolved actinide source term.

b – DOE did not develop a solubility model for the +VI actinides. Consequently, a fixed concentration was assumed for uranium(VI), which is the only +VI actinide predicted to be present in the WIPP repository in significant concentrations.

Table 7-5. Aqueous Actinide Speciation, PABC-2009 FMT Calculations With and Without Organic Ligands*

Aqueous species that constitute more than 2% of the total are indicated in bold.

Brine	GWB		ERDA-6	
	With Ligands	Without Ligands	With Ligands	Without Ligands
Total Americium(III) (M)	1.656×10^{-6}	2.252×10^{-7}	1.514×10^{-6}	8.667×10^{-8}
Am^{3+}	1.240×10^{-11}	1.350×10^{-11}	2.274×10^{-12}	1.792×10^{-12}
$AmOH^{2+}$	2.414×10^{-9}	2.379×10^{-9}	5.851×10^{-10}	4.851×10^{-10}
$Am(OH)_2^+$	$\mathbf{2.114 \times 10^{-7}}$	$\mathbf{2.215 \times 10^{-7}}$	$\mathbf{9.025 \times 10^{-8}}$	$\mathbf{8.487 \times 10^{-8}}$
$Am(OH)_3^0$	6.033×10^{-10}	6.188×10^{-10}	6.930×10^{-10}	7.121×10^{-10}
$AmCO_3^+$	3.734×10^{-10}	3.716×10^{-10}	1.864×10^{-10}	1.696×10^{-10}
$Am(CO_3)_2^-$	1.331×10^{-10}	1.338×10^{-10}	3.023×10^{-10}	3.329×10^{-10}
$Am(CO_3)_3^{3-}$	3.386×10^{-11}	3.322×10^{-11}	7.746×10^{-11}	9.415×10^{-11}
$Am(CO_3)_4^{5-}$	1.049×10^{-11}	9.230×10^{-12}	7.823×10^{-13}	8.654×10^{-13}
$AmAc^{2+}$	2.116×10^{-9}	--	2.975×10^{-10}	--
$AmCit^0$	1.403×10^{-9}	--	5.792×10^{-10}	--
$AmEDTA^-$	$\mathbf{1.437 \times 10^{-6}}$	--	$\mathbf{1.421 \times 10^{-6}}$	--
$AmOx^+$	2.327×10^{-11}	--	3.246×10^{-12}	--
Total Thorium(IV) (M)	5.626×10^{-8}	5.642×10^{-8}	6.982×10^{-8}	7.196×10^{-8}
$Th(OH)_4^0$	$\mathbf{4.515 \times 10^{-8}}$	$\mathbf{4.528 \times 10^{-8}}$	$\mathbf{4.762 \times 10^{-8}}$	$\mathbf{4.774 \times 10^{-8}}$
$Th(OH)_3CO_3^-$	$\mathbf{1.111 \times 10^{-8}}$	$\mathbf{1.113 \times 10^{-8}}$	$\mathbf{2.220 \times 10^{-8}}$	$\mathbf{2.421 \times 10^{-8}}$
$Th(CO_3)_5^{6-}$	4.019×10^{-16}	2.742×10^{-16}	1.925×10^{-17}	1.796×10^{-17}
$ThAc_2^{2+}$	2.631×10^{-20}	--	7.384×10^{-21}	--
$ThCit^+$	1.679×10^{-19}	--	9.825×10^{-20}	--
$ThEDTA^0$	6.169×10^{-17}	--	2.834×10^{-17}	--
$ThOx^{2+}$	1.161×10^{-22}	--	0.00	--
Total Neptunium(V) (M)	3.905×10^{-7}	2.209×10^{-7}	8.746×10^{-7}	5.379×10^{-7}
NpO_2^+	$\mathbf{1.168 \times 10^{-7}}$	$\mathbf{1.156 \times 10^{-7}}$	$\mathbf{1.437 \times 10^{-7}}$	$\mathbf{1.190 \times 10^{-7}}$
NpO_2OH^0	4.081×10^{-9}	4.160×10^{-9}	9.411×10^{-9}	8.687×10^{-9}
$NpO_2(OH)_2^-$	5.974×10^{-12}	6.114×10^{-12}	2.602×10^{-11}	2.622×10^{-11}
$NpO_2CO_3^-$	$\mathbf{9.843 \times 10^{-8}}$	$\mathbf{1.000 \times 10^{-7}}$	$\mathbf{3.994 \times 10^{-7}}$	$\mathbf{3.988 \times 10^{-7}}$
$NpO_2(CO_3)_2^{3-}$	1.126×10^{-9}	1.141×10^{-9}	9.811×10^{-9}	$\mathbf{1.129 \times 10^{-8}}$
$NpO_2(CO_3)_3^{5-}$	1.339×10^{-11}	1.293×10^{-11}	7.788×10^{-11}	9.517×10^{-11}
NpO_2Ac^0	$\mathbf{1.324 \times 10^{-7}}$	--	$\mathbf{2.593 \times 10^{-7}}$	--
NpO_2Cit^{2-}	4.302×10^{-10}	--	2.006×10^{-9}	--
NpO_2EDTA^{3-}	3.470×10^{-12}	--	3.805×10^{-12}	--
NpO_2Ox^-	$\mathbf{3.719 \times 10^{-8}}$	--	$\mathbf{5.087 \times 10^{-8}}$	--
Output File Name	FMT_PABC09_ GWB_HMAG_ ORGS_005.OUT	FMT_PABC09_ GWB_HMAG_ NOORGS_006. OUT	FMT_PABC09_ E6_HMAG_ ORGS_013.OUT	FMT_PABC09_ E6_HMAG_ NOORGS_014. OUT

* All americium-sulfate and americium-chloride aqueous complexes [$AmCl^{2+}$, $AmCl_2^+$, $AmSO_4^+$, $Am(SO_4)^-$] and all thorium-sulfate aqueous complexes [$Th(SO_4)_2^0$, $Th(SO_4)_3^{2-}$] were present at negligible concentrations. Only the highest-concentration actinide-organic ligand aqueous species are listed.

7.2   COLLOIDAL ACTINIDE SOURCE TERM

The Colloidal Actinide Source Term conceptual model was peer reviewed prior to the CCA PA and PAVT and found to be adequate (Wilson et al. 1996a). This conceptual model and its implementation were the same in the CCA PAVT, PABC04, CRA-2009 PA and PABC09.

It has been assumed that four types of colloids can form in the WIPP repository and influence the Actinide Source Term:

- Microbial colloids
- Humic colloids
- Intrinsic colloids
- Mineral fragment colloids

The concentrations of actinide intrinsic colloids and mineral fragment colloids used in PA are constant values (Table 7-6). The concentrations of intrinsic plutonium(IV) colloids were determined based on the results of experimental investigations carried out with plutonium(IV) (DOE 1996b, Appendix SOTERM, Section 6.3.2.3; Papenguth and Behl 1996). A literature review did not provide evidence of the formation of other actinide intrinsic colloids, so the concentrations of thorium, uranium, neptunium, plutonium(III) and americium intrinsic colloids were set equal to zero (DOE 1996b, Appendix SOTERM, Section 6.3.2.4). However, more recent investigations (Neck et al. 2002; Bitea et al. 2003; Altmaier et al. 2004) identified the formation of intrinsic thorium colloids in dilute solution and in brines. EPA (2010e) found that although the formation of thorium intrinsic colloids could not be ruled out on the basis of the available evidence, formation of these intrinsic thorium colloids would not have significant effects on repository performance.

Table 7-6.   Actinide Concentrations Associated with Mineral Fragment and Intrinsic Colloids

	Mineral Fragment Colloids (M)	Intrinsic Colloids (M)
Thorium(IV)	2.6×10^{-8}	0.0
Uranium(IV)	2.6×10^{-8}	0.0
Uranium(VI)	2.6×10^{-8}	0.0
Neptunium(IV)	2.6×10^{-8}	0.0
Neptunium(V)	2.6×10^{-8}	0.0
Plutonium(III)	2.6×10^{-8}	0.0
Plutonium(IV)	2.6×10^{-8}	1.0×10^{-9}
Americium(III)	2.6×10^{-8}	0.0

Source: DOE 1996b, Appendix SOTERM, Table SOTERM-14

Altmaier et al. (2004) also determined that mineral fragment colloids formed in $MgCl_2$ solutions with an ionic strength from 2.5 to 4.5 M, and that these colloids can mobilize higher concentrations of thorium than the concentrations used in WIPP PA (Table 7-6). DOE provided evidence that the mineral fragment colloids identified by Altmaier et al. (2004) would not be stable in WIPP brine. EPA (2010e) concurred that these colloids would not be expected to form or persist in the WIPP repository environment. Consequently, the thorium concentration associated with mineral fragment colloids was appropriate for the PABC09. However, EPA

(2010e) noted that mineral-fragment colloid formation had not been investigated with MgO hydration and carbonation products and recommended such an investigation be conducted before the CRA-2014.

Actinide concentrations associated with humic substances are based on proportionality constants (Table 7-7). Proportionality constants determined for thorium(IV) were extended to uranium(IV), neptunium(IV) and plutonium(IV), and proportionality constants developed for americium(III) were extended to plutonium(III). Proportionality constants for neptunium(V) and uranium(VI) were based on data for these oxidation states (DOE 1996b, Appendix SOTERM, Table SOTERM-12). The proportionality constants were calculated from experimentally determined humic substance solubilities in brines at various concentrations of Ca^{2+} and Mg^{2+}; data on site-binding capacities measured for the WIPP research program and literature values; actinide complexation factors for americium(III), thorium(IV), neptunium(V) and uranium(VI) binding on humic substances; and stability constants for Ca^{2+} and Mg^{2+} binding to humic substances. The maximum value used in PA (CAPHUM, Table 7-7) represents the theoretical maximum concentration of actinides that can be bound by a humic substance, assuming a solubility limit of 2 mg/liter, the highest site-binding capacity for fulvic acids of 5.56 meq OH^-/g and the limiting case of a monovalent actinide species (DOE 1996b, Appendix SOTERM, Section 6.3.3.2).

Actinide concentrations associated with microbial colloids are also based on proportionality constants (Table 7-7). For microbes, the proportionality constant is related to the actinide element, rather than the oxidation state. Experimental data on the mobile concentrations of microbes and bioaccumulation and toxicity experiments were used to develop the proportionality constants. Upper limits for the concentrations of actinides for microbial colloids were established based on the concentration at which no growth was observed (Table 7-7). Because of the high radiation levels of americium, no maximum concentration value was determined for americium. Because of limited data, distributions were not developed for the proportionality constants or the maximum concentrations for microbial colloids, and single values were used in PA (DOE 1996b, Appendix SOTERM, Section 6.3.4.2).

Table 7-7. **Proportionality Constants and Maximum Concentrations for Humic and Microbial Colloids**

	Proportionality Constant Humic Colloids in Salado Brine[a]	Proportionality Constant Humic Colloids in Castile Brine[b]	Maximum Sorbed on Humics (M)	Proportionality Constant Microbes[a]	Maximum Sorbed by Microbes[c]
Parameter	PHUMSIM	PHUMCIM	CAPHUM	PROPMIC	CAPMIC
Thorium(IV)	6.3	6.3	1.1×10^{-5}	3.1	0.0019
Uranium(IV)	6.3	6.3	1.1×10^{-5}	0.0021	0.0021
Uranium(VI)	0.12	0.51	1.1×10^{-5}	0.0021	0.0023
Neptunium(IV)	6.3	6.3	1.1×10^{-5}	12.0	0.0027
Neptunium(V)	9.1×10^{-4}	7.4×10^{-3}	1.1×10^{-5}	12.0	0.0027
Plutonium(III)	0.19[d]	1.37[d]	1.1×10^{-5}	0.3	6.8×10^{-5}
Plutonium(IV)	6.3	6.3	1.1×10^{-5}	0.3	6.8×10^{-5}
Americium(III)	0.19[d]	1.1[d]	1.1×10^{-5}	3.6	NA[e]

a – Units of moles colloidal actinide per mole dissolved actinide
b – Units of moles colloidal actinide per mole dissolved actinide
c – Units of moles total mobile actinide per liter
d – For Salado brine, the maximum value in the distribution is used for PA; for Castile brine, a cumulative
   distribution from 0.065 to 1.60 with a mean value of 1.1 and a median of 1.37 is sampled for PA
e – Not applicable
Source: DOE 1996b, Appendix SOTERM, Table SOTERM-14

The parameter values for the colloidal actinides in Tables 7-6 and 7-7 have been used in all
WIPP PA calculations since the CCA PA. EPA (2010e) reviewed the available information
regarding colloidal actinide transport and determined that the effects of colloidal transport were
adequately accounted for in the PABC09. However, EPA (2010e) recommended that DOE
should investigate the potential formation of intrinsic thorium colloids and the potential
formation of mineral fragment colloids from MgO hydration and carbonation products for the
CRA-2014.

7.3   EFFECTS OF DISSOLVED ACTINIDE SOLUBILITY AND COLLOIDAL ACTINIDE CHANGES ON PABC09 RESULTS

The calculated actinide solubilities used in the PABC04 and PABC09 are higher than the
solubilities used in the CCA PAVT (Table 7-8). The increased concentrations of the +III
actinides were primarily caused by increased inventories of organic ligands. Smaller increases in
the +IV actinide solubilities resulted from changes in the thorium(IV) data in the FMT database
since the CCA PAVT. Thorium(IV) and neptunium(V) concentrations are predicted to be
controlled by the solubilities of $ThO_2(am)$ and $KNpO_2CO_3(s)$, respectively, which has remained
unchanged since the CCA PAVT. For the CCA PAVT, $AmOHCO_3(cr)$ was predicted to be the
solubility-controlling solid for the +III actinides. As a result of revisions to the FMT database
between the CCA PAVT and the PABC04, $Am(OH)_3(s)$ was predicted to be the solubility-
controlling solid phase for the PABC04 and PABC09.

Table 7-8. Actinide Solubility Calculations for the CCA PAVT, the PABC04 and the PABC09

Property or Actinide Oxidation State	CCA PAVT No Organic Ligands		PABC04 With Organic Ligands		PABC09 With Organic Ligands	
Brine	Salado (Brine A)	Castile (ERDA-6)	Salado (GWB)	Castile (ERDA-6)	Salado (GWB)	Castile (ERDA-6)
pH	8.69	9.24	8.69	8.94	8.69	8.98
pcH	--	--	9.39	9.64	9.40	9.68
Log CO_2 fugacity	-5.50	-5.50	-5.50	-5.50	-5.50	-5.50
Total Carbon (M)	--	--	2.16×10^{-5}	5.18×10^{-5}	3.50×10^{-4}	4.48×10^{-4}
III (M)	1.2×10^{-7}	1.3×10^{-8}	3.87×10^{-7}	2.88×10^{-7}	1.66×10^{-6}	1.51×10^{-6}
IV (M)	1.3×10^{-8}	4.1×10^{-8}	5.64×10^{-8}	6.79×10^{-8}	5.63×10^{-8}	6.98×10^{-8}
V (M)	2.4×10^{-7}	4.8×10^{-7}	3.55×10^{-7}	8.24×10^{-7}	3.90×10^{-7}	8.75×10^{-7}
VI (M)[a]	8.7×10^{-6}	8.8×10^{-6}	10^{-3}	10^{-3}	10^{-3}	10^{-3}
Equilibrium Nonradionuclide Solid Phases	Anhydrite, halite, brucite, hydromagnesite, korshunovskite	Anhydrite, halite, brucite, glauberite, hydromagnesite	Anhydrite, halite, brucite, hydromagnesite, whewellite, korshunovskite	Anhydrite, halite, brucite, hydromagnesite, whewellite, glauberite	Anhydrite, halite, brucite, hydromagnesite, whewellite, korshunovskite	Anhydrite, halite, brucite, hydromagnesite, whewellite, glauberite
Equilibrium Radionuclide Solid Phases	$AmOHCO_3(cr)$, $ThO_2(am)$, $KNpO_2CO_3(s)$		$Am(OH)_3(s)$, $ThO_2(am)$, $KNpO_2CO_3(s)$,		$Am(OH)_3(s)$, $ThO_2(am)$, $KNpO_2CO_3(s)$,	
FMT Database	FMT_970407.CHEMDAT		FMT_050405.CHEMDAT		FMT_050405.CHEMDAT	
FMT output filename	--	--	FMT_CRA1BC_ GWB_HMAG_ ORGS_007	FMT_CRA1BC_ ER6_HMAG_ ORGS_007	FMT_PABC09_ GWB_HMAG_ ORGS_005.OUT	FMT_PABC09_E6_ HMAG_ORGS_013. OUT

a – DOE did not develop a solubility model for the +VI actinides. Therefore, for all PAs, a fixed concentration was assumed for uranium(VI), which is the only +VI actinide predicted to be present in the WIPP repository in significant concentrations.

Increased concentrations of dissolved actinides in the PABC09 resulted in higher colloid concentrations than predicted for the CCA PAVT, because actinides associated with humic and microbial colloids are proportional to the dissolved actinide concentrations (Table 7-7). EPA (2010e) calculated the concentrations of dissolved and colloidal actinides using mean values of all sampled parameters. Because the constant concentrations of mineral fragment colloids and intrinsic colloids are relatively low, contributions of these types of colloids to the total mobile actinides are low for all actinide oxidation states for the mean PABC09 case. In GWB brine, the majority of the total mobilized actinides are colloidal, except for plutonium(III) and uranium(VI). For ERDA-6 brine, only uranium(VI) dominates the dissolved fraction of the total mobilized concentration. These results demonstrate that the Colloidal Actinide Source Term conceptual model and its implementation significantly influence predicted total mobilized actinide concentrations.

7.4 CONCLUSIONS REGARDING PABC09 DISSOLVED AND COLLOIDAL ACTINIDE SOURCE TERMS

The available data support the assumption that the MgO backfill will adequately control brine pH and CO_2 fugacities, and thereby limit actinide solubilities in WIPP brines under inundated conditions. The assumptions related to actinide oxidation states in the WIPP repository have remained unchanged since they were developed and peer reviewed for the CCA. It is assumed that thorium(IV), americium(III) and curium(III) are the only oxidation states that will be present in the WIPP repository for these radionuclides. It is assumed that plutonium may be present in the +III or +IV oxidation states, neptunium may be present in the +IV or +V oxidation states, and uranium may be present in the +IV or +VI oxidation states. Because of the reducing conditions that will be established in the repository shortly after closure, these oxidation state assumptions were appropriate for the PABC09.

DOE (2009, Appendix SOTERM-2009) provided a qualitative review of actinide solubility and speciation data relevant to WIPP brines that became available since the PABC04, but did not revise the FMT database for the PABC09 actinide solubility calculations. EPA (2010e) reviewed the actinide solubility and aqueous speciation data that have become available since the most recent revision of the FMT database and determined that the actinide solubilities calculated using this database were adequate for use in the PABC09. EPA (2010e) also reviewed the development of the +III and +IV actinide solubility uncertainty distributions and the colloidal actinide source term calculations and determined that these calculations were adequate for the PABC09.

8.0   CULEBRA FLOW AND TRANSPORT

8.1   INTRODUCTION

In the CRA-2009 and PABC-2009, the Culebra member of the Rustler Formation is conceptualized as a horizontal, confined aquifer of uniform density. For fluid flow, the Culebra is assumed to be a heterogeneous porous medium with spatially varying transmissivity (T). A heterogeneous velocity field is also assumed to be used for radionuclide transport, but all other rock properties are conceptualized as constant (homogeneous) across the model area. The Culebra is conceptualized as having two types of porosity; a portion of the porosity is associated with high-permeability features where transport occurs by advection, and the rest of the porosity is associated with low-permeability features where flow does not occur and retardation occurs by physical processes (diffusion) and chemical processes (sorption). This type of conceptual model is commonly referred to as double-porosity.

The key factors controlling fluid flow in the Culebra are the hydraulic gradient, transmissivity distribution and porosity. In the Culebra conceptual model, the spatial distribution of transmissivity is important. The hydraulic gradient and transmissivities used in PA are coupled, because they are calibrated to observed conditions. It is possible that radionuclides might be introduced into the Culebra through brine leakage around shaft seals. However, the chief source of actinides in the Culebra is long-term releases from an inadvertent intrusion borehole that intersects the repository. If radionuclides are introduced into the Culebra, they may be transported from the point of introduction by groundwater flowing naturally through the Culebra.

In the CRA-2009 and PABC-2009, radionuclide transport in the Culebra was modeled by the following steps:

(1) Constructing conditioned geostatistical realizations of Culebra hydraulic transmissivity fields (T-fields)

(2) Modifying the T-fields to account for potential subsidence due to potash mining in formations beneath the Culebra

(3) Calculating steady-state groundwater flow fields for each mining-modified T-field

(4) Calculating radionuclide transport through the Culebra for each flow field

Culebra transport simulations calculate the cumulative discharge at the land withdrawal boundary over the 10,000-year regulatory period due to a source located at the center of the waste panel area.

Many additional Culebra transmissivity datasets are now available, compared with the information utilized to generate the transmissivity fields (T-fields) used in the CRA-2009 PA (Beauheim 2010). Additional locations near the WIPP site have been tested and long-term pumping tests have been performed. The additional datasets and modified conceptual model were used for the PABC-2009 T-field calibration. Furthermore, the additional datasets were used to calculate parameters used to represent the Culebra and Magenta properties in the Salado

flow calculations (Beauheim 2009). Table 8-1 lists the Culebra and Magenta parameters that were updated to include this information.

Table 8-1.   Culebra and Magenta Parameters Modified for the PABC-2009

Description	Materials	Properties
Brine far-field pore pressure	CULEBRA, MAGENTA	PRESSURE
Log of intrinsic permeability	CULEBRA, MAGENTA	PRMX_LOG, PRMY_LOG, PRMZ_LOG

In the PABC-2009, DOE relates the observed Culebra transmissivities (T) to the following deterministic factors: the thickness of overburden above the Culebra, the presence or absence of dissolution of the upper Salado, and the presence or absence of halite in units above and below the Culebra. Culebra T is also related to the occurrence of open, interconnected fractures that cannot be mapped as easily as the other three factors and, therefore, DOE treats fracture properties stochastically. DOE developed a linear-regression model for Culebra T based on these factors to create 1,000 stochastic realizations of the distribution of Culebra T ("base" T-fields) in the vicinity of the WIPP site.

DOE has applied the groundwater flow code, MODFLOW-2000, to simulate flow within the Culebra. The modeling domain was defined extending 30.7 km north-south and 28.4 km east-west, roughly centered on the WIPP site. This domain was discretized into 87,188 uniform 100-m square two-dimensional finite-difference cells. An inactive portion of the northwest corner of the domain is used to represent a no-flow boundary in the axis of Nash Draw. A low-permeability constant-head portion of the eastern section of the domain is used to represent the lithostatic portion of the Culebra sandwiched above and below by halite units. Freshwater head observations in 42 monitoring wells from May 2007 were used as steady-state calibration targets. Drawdown observations in 62 observation wells, in response to 9 unique pumping tests, were used as transient calibration targets. A subset consisting of 100 of the 200 calibrated Culebra model realizations was selected based on their ability to simulate these observed heads.

The Agency requires that the potential effects of future potash mining be taken into account when evaluating the performance of the WIPP disposal system. Accordingly, DOE has scaled the transmissivities in the areas within the model domain where current or future mining might affect the Culebra by a random multiplier between 1 and 1,000. A single multiplier was used for each T-field, applied first to the areas outside the WIPP LWB that might be mined to create a partial mining T-field, and then to all areas (both inside and outside the WIPP LWB) to create a full mining T-field. Three statistically similar replicates of mining multipliers were generated, leading to a total of 600 unique T-fields (100 calibrated realizations, 2 mining scenarios and 3 replicates). The MODFLOW-2000 flow budgets were used from each T-field as input for both advective particle tracking (DTRKMF) and radionuclide solute transport (SECOTP2D).

The non-mined travel times from the center of the WIPP waste panels to the WIPP LWB are similar to those computed for the CCA, and therefore faster than those computed for the PABC-2004. The decrease in travel time to the LWB can be attributed to the presence of a consistent high-transmissivity pathway leaving the south-east portion of the LWB. The presence of this pathway is supported by observed drawdown data from the SNL-14 pumping test. In the partial-mining case, particle tracks show increased travel times from the center of the WIPP waste

panels to the WIPP LWB, compared to the non-mining scenario. In the full-mining case, particle tracks showed decreased travel times to the WIPP LWB, due to the close proximity of minable potash to the center of the WIPP waste panels.

8.2   CONCEPTUAL MODEL DEVELOPMENT AND PEER REVIEW

The Culebra hydrology conceptual model describes the overall hydrogeologic framework of the Culebra Dolomite Member of the Rustler Formation in the vicinity of the WIPP site. The Culebra stratigraphic unit is the most significant potential groundwater transport pathway for radionuclides released from the WIPP repository. The original conceptual model for Culebra hydrogeology developed for the CCA was found to be inadequate by the Conceptual Models Peer Review Panel, because a strong correlation was not established between the conceptual model and the numerical model used in PA. Although the original conceptual model was inadequate, this was of little consequence, because release of radionuclides through the Culebra was very limited.

In response to these concerns, the DOE revised the Culebra hydrology model to establish a stronger link between the Culebra hydrogeology and the numerical hydrogeologic model. As part of this process, the DOE also sought to improve the ability of the model to reproduce the observed hydrologic behavior of the Culebra with respect to fluid flow.

Once the DOE completed their revision to the Culebra hydrology conceptual model (identified as the RCHCM), it was subjected to another peer review (Burgess et al. 2008). The scope of the peer review was limited to Culebra flow modeling; transport modeling is handled by a separate PA model and was not included in the Panel's scope. The Panel reviewed sedimentological, geochemical, hydrologic, numerical simulations and geostatistical information that the DOE integrated to form the conceptual model. The Panel also reviewed the method by which that information was used to develop calibrated T-fields. In its assessment of the validity of conclusions reached through use of the conceptual model, the Peer Panel made the following statement:

> *The Panel believes that the conclusions in the RCHCM from the integration of geology and hydrology are valid, and can be used to develop T-fields for incorporation in the PA.*

As discussed in EPA (2008), the Agency agreed with the Panel's conclusion on the basis of the rationale presented in the Panel's report, and also on the basis of the demonstrated improvement in the ability of the RCHCM to be calibrated to measured heads and transient field test results over that of the previous Culebra flow model.

The geology and geologic history of the Culebra has been described in the literature (Holt and Powers 1988; Beauheim and Holt 1990; Holt 1997). The RCHCM of the Culebra dolomite located in the area of the WIPP site is developed from these references and is shown in Figure 8-1. Specifically, the RCHCM follows assumptions detailed in Holt (1997) that assume that the variability in Culebra transmissivity is due strictly to post-depositional processes. To

better quantify the RCHCM, Beauheim (2010) identifies geologic controls on Culebra transmissivity and develops a linear mathematical model relating these controls to transmissivity.

Except for the mining scenarios, transmissivity was assumed to be constant over time. A number of significant changes have been made since the PABC-2004 with respect to the calculation of the transmissivity fields and are presented in the sections that follow.
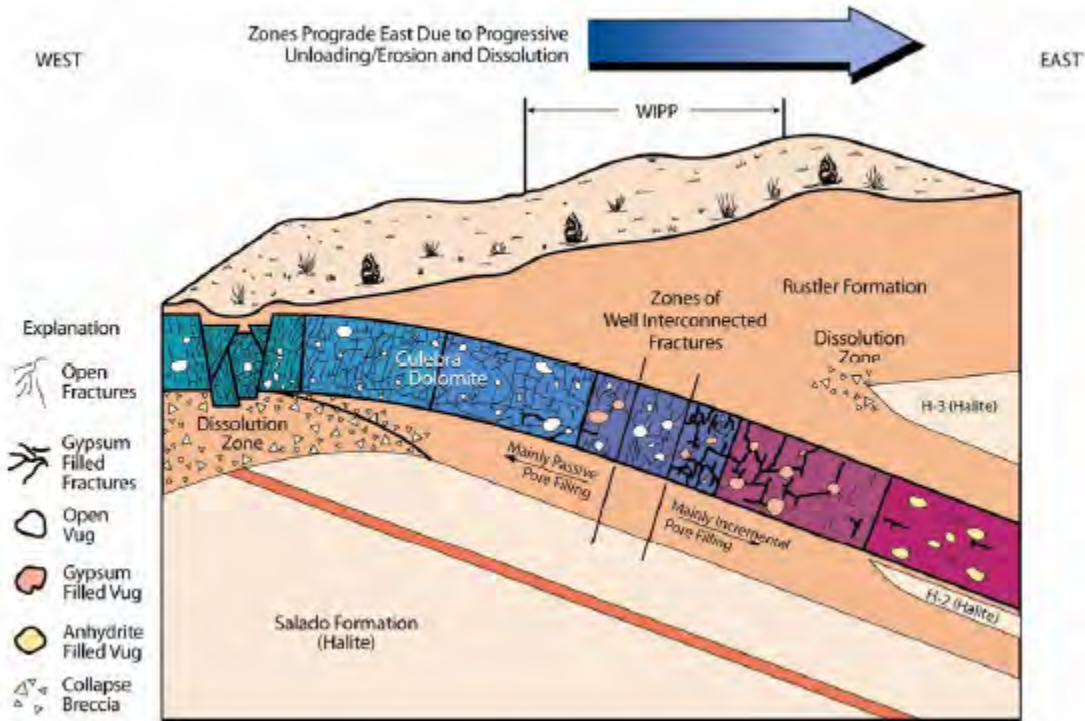

Figure 8-1.   Culebra Dolomite Conceptual Model near WIPP

Culebra T values decrease to the east (increasing overburden and halite), and fracturing increases to the west (Salado dissolution zone). Halite appears both above (H-3) and below (H-2) the Culebra in the east (Beauheim 2010).

8.3   DEVELOPMENT OF THE TRANSMISSIVITY FIELDS

8.3.1   Summary of Approach

DOE's starting point in the T-field development process was to assemble and update information on geologic factors that might affect Culebra transmissivity. These factors include dissolution of the upper Salado Formation, the thickness of overburden above the Culebra, fracture interconnection, and the spatial distribution of halite in the Rustler Formation both above and below the Culebra. After the data were assembled and updated, DOE applied a two-part "geologically based" approach to generate Culebra base T-fields. In the first part, the conceptual model for geologic controls on Culebra T was formalized, and the hypothesized geologic controls were regressed against measured Culebra T data to determine linear regression coefficients. The regression includes one continuously varying function, Culebra overburden

thickness and three indicator functions that assume values of 0 or 1 depending on the occurrence of open, interconnected fractures, Salado dissolution, and the presence or absence of halite in units bounding the Culebra.

In the second part of the analysis, a method was developed for applying the linear regression model to predict Culebra T across the WIPP area. The regression model was combined with the maps of geologic factors to create 1,000 stochastically varying Culebra base T-fields. The development of the regression model and the creation of the base T-fields are summarized in the sections that follow and additional details are provided in Hart et al. (2008).

DOE used several types of "soft data" to also constrain the stochastic simulation, including halite in the Rustler, the presence of gypsum cements in the Rustler, and diffusivity values obtained from hydraulic tests. The indicator kriging process for including soft data is detailed in Hart et al. (2008).

T-fields were calibrated to both steady-state heads and transient drawdown measurements. Heads measured in 42 observation wells around May 2007 were used to represent steady-state conditions in the Culebra, and drawdown responses in 67 total observation wells (62 unique locations) across 9 pumping tests were used to provide transient calibration data. Details on the steady-state heads are described in Johnson (2009), and the transient drawdown data are summarized in Hart et al. (2008).

Development of Geologic Model

Significant changes have been made to the T-field development since the PAVT. In the PAVT, the computer code GRASP_INV relied solely upon measured transmissivities and water levels to predict the T-fields. DOE's most recent approach for CRA-2009 and PABC-2009, however, incorporates geologic information that affects the transmissivity. These factors include dissolution of the upper Salado Formation, the thickness of overburden above the Culebra, fracture interconnection and the spatial distribution of halite in the Rustler Formation above and below the Culebra. DOE obtained this geologic information from hundreds of oil and gas wells and potash exploration holes in the vicinity of the WIPP site. In addition, T values are available from only 64 well locations. Details of the geologic data compilations are given in (Powers 2002, 2003), updated in Powers (2007). DOE has made significant changes to the locations of the halite margins in some areas since CRA-2004. The Rustler halite margins defined in Powers (2007) are used by Beauheim (2010) in the development of the T-fields.

DOE hypothesizes that Culebra transmissivity is inversely related to thickness of overburden because stress relief associated with erosion of overburden leads to fracturing and opening of pre-existing fractures. Culebra transmissivity is observed to be high where dissolution of the upper Salado has occurred and the Culebra has subsided and fractured. Culebra transmissivity tends to be low where halite is present in overlying and/or underlying mudstones. DOE has assumed that high Culebra transmissivity leads to dissolution of nearby halite (if any). From this assumption, DOE concludes that the presence of halite in mudstones above and/or below the Culebra can be taken as an indicator for low Culebra transmissivity. Based upon the distribution

of measured values of transmissivity in relation to overburden maps, the Agency believes that DOE's assumptions are reasonable.

The Culebra transmissivity data used in the PABC-2009 modeling are the same as those used by Holt and Yarbrough (2002), supplemented by more recent data reported from recent pumping tests (Roberts 2006; Roberts 2007; Bowman and Roberts 2009). The log transmissivity data show a bimodal distribution. As closely spaced wells can show very different values, DOE hypothesizes that higher transmissivity values reflect the presence of well-interconnected fractures that are absent at lower transmissivity locations. Well-interconnected fractures occur in regions affected by Salado dissolution (e.g., Nash Draw) and in areas with complicated cement dissolution and precipitation histories (e.g., high-transmissivity zones near the WIPP site). High-transmissivity zones within the Culebra can occur between areas bounded on the west by the Salado dissolution margin and bounded on the east by halite present in the Tamerisk and Los Medanos members. In these zones, fractures are well interconnected, and fracture interconnectivity is controlled by a complicated history of fracturing with several episodes of cement precipitation and dissolution (Beauheim and Holt 1990; Holt 1997). DOE has not been able to correlate fracture interconnectivity to other geologic features in cores or from subsurface geophysical logs, and fracture interconnectivity can only be identified from in situ hydraulic test data.

Because of this lack of a geologic correlation, DOE considers the spatial location of high-transmissivity zones to be a stochastic process that cannot be predicted deterministically. Instead, DOE creates these fractured zones by using geostatistical indicator kriging with conditioning data. This is a change from the approach applied in PABC-2004 (Holt and Yarbrough 2002), where the only conditioning information was based on the known T values at wells. For the PABC-2009 analysis, DOE has added information to the geostatistical model to increase the likelihood of high T being placed between two wells that hydraulic testing has shown to be well connected. Likewise, areas where there is evidence of high levels of gypsum (i.e., low permeability) are given a slightly lower probability of being in a high T zone. This allows DOE to merge both hydraulic and geologic data in the creation of high T zones, while still keeping zone placement and shape a stochastic process.

Relationship of Transmissivity to Geologic Properties

Holt and Powers (1988), Powers and Holt (1990), Beauheim and Holt (1990) and Holt (1997) have described the geology and geologic history of the Culebra. DOE developed several geologically based relationships from this work by assuming that variability in transmissivity is due strictly to post-depositional processes. The Agency has also reviewed this work and has concluded that the majority of the existing evidence (e.g., post-depositional precipitation of gypsum within the Culebra) supports DOE's conclusion.

As discussed above, DOE has assumed that the spatial distribution of transmissivity on a regional scale is a function of a series of deterministic geologic controls, including Culebra overburden thickness, fracture interconnection, dissolution of the upper Salado Formation and the occurrence of halite in units above or below the Culebra. Geologic maps were developed to determine these controls at any location. In the region between the margin of upper Salado

dissolution and the margin of halite occurrence above the Culebra (which includes the WIPP site), however, high-T regions occur that cannot be predicted using geologic data. This is because no geologic metric has yet been defined that allows prediction of where fractures are filled or open, and therefore knowledge of this indicator east of the Salado dissolution margin is limited to the test well locations. DOE treats these high transmissivity zones stochastically.

The second major step in the development of the T-field involved regression of the three hypothesized geologic controls against Culebra transmissivity data to determine linear regression coefficients. The regression includes one continuously varying function, Culebra overburden thickness, and three indicator functions that assume values of 0 or 1 depending on the occurrence of open, interconnected fractures, Salado dissolution, and the presence or absence of halite in units bounding the Culebra.

The fracture interconnection relationship is based on a bi-modal assumption of Culebra transmissivity, which is correlated to the degree that the fractures are filled with gypsum. The Agency believes that this assumption is reasonable, based upon work conducted by Beauheim and Ruskauff (1998) and Holt (1997). Other major assumptions in DOE's regression analysis (e.g., an inverse relationship exists between Culebra overburden thickness and T) also appear to provide a reasonable means to establish correlations from which the transmissivity can be estimated.

Once the correlations were established, DOE developed a linear-regression model using the Windows®-based program Mathcad 7 Professional (Hart et al. 2008). Although other variables are input, this model requires only $\log_{10} T$ data from tested wells, the depth of the Culebra at those wells, and an estimate of whether dissolution of the upper Salado has or has not occurred at each location. The fracture interconnectivity indicator is defined from the $\log_{10} T$ data, and a Salado dissolution indicator is defined using the Salado dissolution data. These data are then used in a standard linear regression algorithm to determine the regression coefficients. This aspect of DOE's effort is relatively standard with respect to regression analyses, and the Agency is in agreement with the general approach.

Calculation of Base Transmissivity Fields

After DOE established the regression coefficients, a geostatistical approach was used to generate 1,000 equally probable realizations of zones with hydraulically significant fractures in the WIPP region (Hart et al. 2009). These simulations were parameterized using the frequency of occurrence of WIPP wells with hydraulically significant fractures and a fit to a variogram constructed using data from those same wells. The regression model was then applied to the entire WIPP area by:

(1) Overlaying the geologic map data for Culebra overburden thickness, Salado dissolution, and the presence or absence of halite in units bounding the Culebra with each of the 1,000 equally probable realizations of zones containing open, interconnected fractures

(2) Sampling each grid point within the model domain to determine the overburden thickness and the indicator values for Salado dissolution, overlying or underlying halite, and fracture interconnectivity

(3) Using the sampled data at each grid point with the regression model coefficients to estimate transmissivity

When applied to the 1,000 equally probable realizations of zones containing open, interconnected fractures, this procedure generates 1,000 stochastically varying Culebra base T-fields.

The base T-fields rely on a regression model to estimate T at every location. It is the nature of regression model that the estimated T values will not honor the measured T values at the measurement locations. Therefore, before using these base T-fields in a flow model, they must be conditioned to the measured T values. DOE performs this conditioning with a Gaussian geostatistical simulation algorithm to generate a series of 1,000 spatially correlated residual fields where each field has a mean value of zero. These fields are conditional, such that the residual value at each measurement location, when added to the value provided by the regression model (which is the same for all 1,000 fields), provides the known T value at that location.

Details about the creation of the base transmissivity fields are provided in Beauheim (2010) and Hart et al. (2008). The Agency reviewed that information and concludes that, although there is some uncertainty associated with DOE's approach, it does include greater amounts of actual data than were used in the development of the T-fields for PABC-2004 (T-fields were based solely on measurements from 46 well locations). It also provides a basis for the development of a conceptual model for the Culebra T-fields, which was lacking in the PABC-2004.

Calibration to Steady-State and Transient Heads

This section presents details on the modeling approach used to calibrate the T-fields to both the May 2007 steady-state heads and the drawdown data collected during 9 independent multi-well pumping tests over more than 20 years. All of these steps outlined below can be considered as preprocessing aspects of the stochastic inverse calibration procedure also discussed below. The actual calibrations are done using an iterative coupling of the MODFLOW-2000 and PEST codes. The details of this process are covered in Hart et al. (2009), and are briefly summarized in the sections that follow.

(1) Assumptions made in the modeling and the implications of these assumptions are provided. Major assumptions include:

- The boundary conditions along the model domain boundary are known and do not change over the timeframe of the model.

- The fracture permeability of the Culebra can be adequately modeled as a continuum at the 100-m $\times$ 100-m grid block scale, and the measured T values used to condition the model are representative of the T in the 100-m $\times$ 100-m grid block in which the well test was performed.

- Variable fluid densities in the Culebra can be adequately represented by casting the numerical solution in terms of freshwater head. Davies (1989) investigated the effects of variable fluid density on the directions of flow calculated in the Culebra

using a freshwater-head approach. Forty-two freshwater head values measured in May 2007 were used for the calibration (Johnson 2009).

All of these assumptions were considered by the Agency during the CCA review and found to be acceptable (EPA 1998b).

An item of particular relevance is that on average, the grid blocks are considerably finer in the PABC-2009 than were used in the PABC-2004. Therefore, there is greater flexibility in the PABC-2009 to accommodate smaller spatial correlation lengths of fracture permeability and T.

(2) The initial heads used for each calibration are estimated at each location in the domain using the 42 heads measured in 2007 (Johnson 2009) in conjunction with kriging and accounting for the regional trend in the head values.

The Agency agrees that the 2007 potentiometric surface data should be used for initial conditions, since earlier datasets are less complete and are not as representative of current conditions. The EPA also accepts kriging as a standard geostatistical method that is often used to contour (i.e., spatially correlate) hydrogeologic data.

(3) The boundary and initial conditions used in the PABC-2009 are described fully in Hart et al. (2009). Regional flow rates within the flow model are controlled by the boundary conditions and the hydraulic conductivity. For the PABC-2009 grid, the constant heads are averaged along the non-halite-sandwiched portion of the northern boundary (943.9 m). In order to obtain the measured gradient, the average heads along the entire southern boundary (911.6 m) are subtracted, and then the difference is divided by the north-south model domain distance (30.7 km). DOE assumes that mining impacts will not significantly change this regional gradient, and thus the specified initial conditions for the mining scenarios are identical to those in Hart et al. (2009).

The CCA, CRA-2004, and PABC-2004 all used this same conceptualization (keeping the outer boundary conditions fixed between the mining and non-mining scenarios); the same conceptualization is maintained to allow for comparisons between the different models. These boundary conditions follow the same basic principles that were accepted by the Agency during the CCA review (EPA 1998b), and remain appropriate for the modeling of the Culebra in the PABC-2009.

(4) The transient head observations for each hydraulic test and each observation well are selected from the database. These heads are plotted as a function of time for each hydraulic test.

Drawdown responses in 67 total observation wells (62 unique locations) across 9 pumping tests from 1985 to 2008 were used to provide transient calibration data.

(5) The spatial and temporal discretization of the model domain.

The eastern limit of the MODFLOW model domain used in the PABC-2009 analysis (Hart et al. 2008) is extended eastward, compared to the MODFLOW domain used in the PABC-2004 analysis. DOE made this change in order to locate the boundary in an area where halite is present in all of the non-dolomite members of the Rustler Formation, simplifying the specification of the eastern model boundary condition. The MODFLOW flow model domain is aligned with the primary compass directions and is areally discretized into 100 m square cells, yielding a model that is 284 cells or 28.4 km wide (east-west) by 307 cells or 30.7 km tall (north-south). As has been the case since the CCA, the Culebra is modeled as a single horizontal layer of uniform 7.75 m vertical thickness.

The Agency believes that the model discretization used in the PABC-2009 provides an appropriate balance between computational requirements and simulating flow at an adequate scale.

The time period assigned by DOE for the transient simulations lasted more than 20 years, beginning in 1985 and ending in 2008. Additionally, a single steady-state calculation was run prior to the transient modeling. The length of this steady-state time period and the date at which it occurs were arbitrarily set to one day occurring from October 14, 1985, to October 15, 1985. These steady-state heads were measured in the year 2007 and were only set to these October dates to provide a steady-state solution prior to the start of any transient hydraulic events.

The method that DOE has used to initialize the transient simulations with steady-state heads and to specify time periods is consistent with standard engineering practices and acceptable to the Agency.

(6) The transient head observations are given relative weights based on the inverse of the maximum observed drawdown in each hydraulic test.

DOE assigns weights to the observed data for each response to every transient hydraulic test to take into account the differences in the responses across the different tests. The weights are calculated as the inverse of the maximum observed drawdown for each hydraulic test. This weighting scheme applies relatively less weight to tests with large drawdowns and relatively more weight to tests with smaller responses. The Agency agrees with weighting of the data so that the overall calibration will not be dominated by trying to reduce the very large residuals that may occur at a few of the observation locations with very large drawdowns.

(7) The locations of the adjustable pilot points are determined using a combination of approaches.

A major development in the field of stochastic inverse modeling has occurred since the T-fields were constructed for the CCA in 1996. Inverse techniques are now capable of

simultaneously determining optimal T values at a large number of pilot points. In the T-fields constructed for the CCA, pilot points were added one at a time and each point was calibrated prior to the addition of the next pilot point. Furthermore, the total number of pilot points was limited to less than or equal to the total number of T observations to avoid numerical instabilities in the solution of the inverse problem. With the techniques now available and implemented in the computer code PEST, it is possible to use many more pilot points than there are T observations and to calibrate these pilot points simultaneously.

Philosophically, the Agency believes that DOE should take advantage of advances in technology as they become available. The Agency is familiar with PEST applications on other EPA-regulated sites and is satisfied with the fundamental principles of the code.

Stochastic Inverse Calibration

The stochastic inverse calibration process uses multiple pre- and post-processor codes in addition to PEST and MODFLOW-2000. The details of the overall numerical approach to the T-field calibration are documented in Hart et al. (2009). In general, the calibration process is run iteratively until at least one of three conditions are met: (1) the number of iterations reaches the maximum allowable number of 15, (2) the objective function reaches a predefined minimum value of 1,000 m^2, or (3) the value of the objective function changes by less than 1% across three consecutive iterations.

At the end of the calibration process, a residual field is created that when added to the base T-field, reproduces the measured T values at the 42 measurement locations and provides a minimum sum of squared errors between the observed and model-predicted heads/drawdowns.

T-Field Acceptance Criteria

DOE's selection criteria for the "best" calibrated fields consisted of comparing the absolute average error of the modeled steady-state heads to a cutoff value, and comparing the absolute average error of the modeled transient responses to a cutoff value. The steady-state and transient criteria were evaluated separately, and only fields that were less than the cutoff value for both sets of tests were selected as the final fields. The final cutoff values used were the mean value of the errors taken across all 200 fields. Using the mean values resulted in a set of 102 fields, so DOE discarded the 2 fields with the largest sum of the 2 metrics.

The Agency believes that the approach adopted by DOE to develop and implement acceptance criteria provides a logical means to evaluate the modeling results.

8.4   CALCULATION OF ADVECTIVE TRAVEL TIME

The advective travel time for a particle released at the center of the WIPP disposal panels in each field was calculated in the same way as was done in PABC-2004 (McKenna and Hart 2003a and 2003b). DOE obtained the travel times using the streamline particle-tracking algorithm implemented in DTRKMF v. 1.0 (Rudeen 2003), assuming a single-porosity medium with a

porosity of 0.16. DTRKMF calculates particle tracks in two or three dimensions for steady-state and time-dependent, variably-saturated flow fields. The particles are tracked cell-by-cell using a semi-analytical solution. DTRKMF directly reads the cell-by-cell flow budget file from MODFLOW-2000 and uses those values to calculate the velocity field. For each calibrated T-field, a final forward run of MODFLOW-2000 was done, and the cell-by-cell fluxes from this run were used as input to DTRKMF to calculate the travel time. These travel times do not, however, represent the actual predicted travel times of solutes, conservative or non-conservative, through the Culebra. Culebra transport modeling treats the Culebra as a double-porosity medium with transport through advective porosity (e.g., fractures) retarded by diffusion into diffusive porosity (e.g., matrix porosity) and by sorption. The travel times are intended only to allow comparison among T-fields. DTRKMF has been evaluated by EPA and found to be acceptable (EPA 2004e).

The Cummulative Distribution Function (CDF) of the 4-m travel times is presented in Figure 8-2. Figure 8-2 also shows the CDF of travel times from the CCA (DOE 1996b) and CRA-2004 (DOE 2004b). The median travel time for the PABC-2009 analysis is slightly greater (about 300 years) than the CCA median time, and, like the CCA, 33% of the fields produce travel times greater than 10,000 years.

In addition to the travel time, DTRKMF provides the particle streamlines. In Figure 8-3 and Figure 8-4, the particle tracks for the 100 final selected fields are presented. Figure 8-3 shows the travel up to the WIPP land withdrawal boundary, with the grayscale color representing the time for the particle to reach that point on the streamline. Figure 8-4 shows the number of fields producing streamlines that pass through a particular cell. In addition, Figure 8-4 shows the streamlines continuing to the model domain boundary.
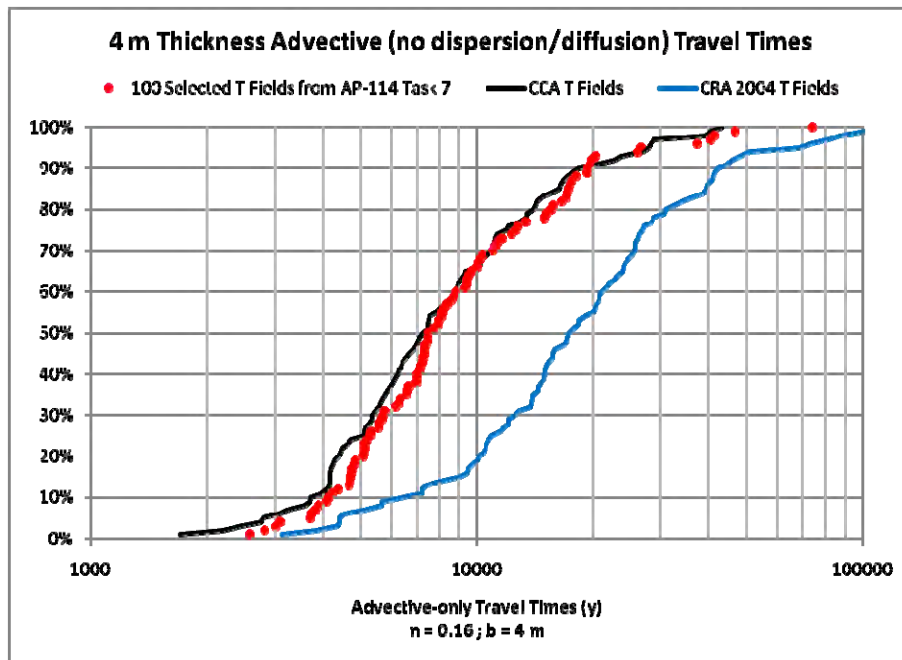

Figure 8-2.   Advective Travel Times to Reach WIPP LWB
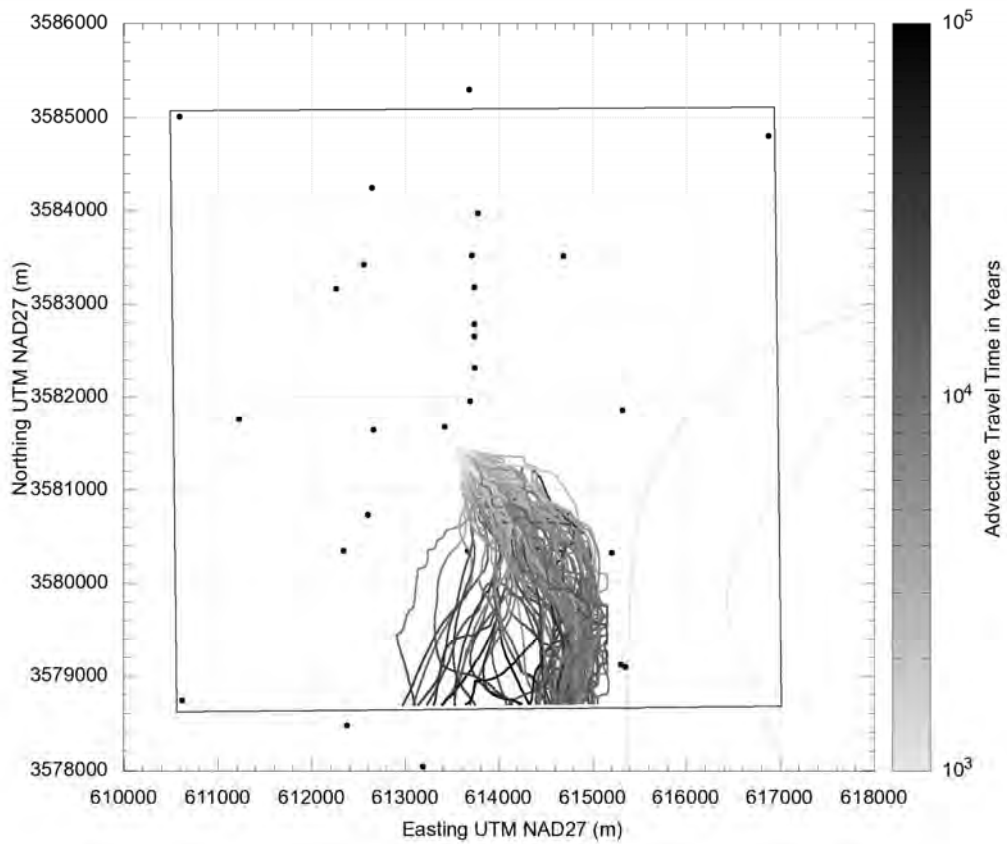
(Hart et al. 2009)

Figure 8-3.   Particle Streamlines to the LWB for the 100 Selected Fields

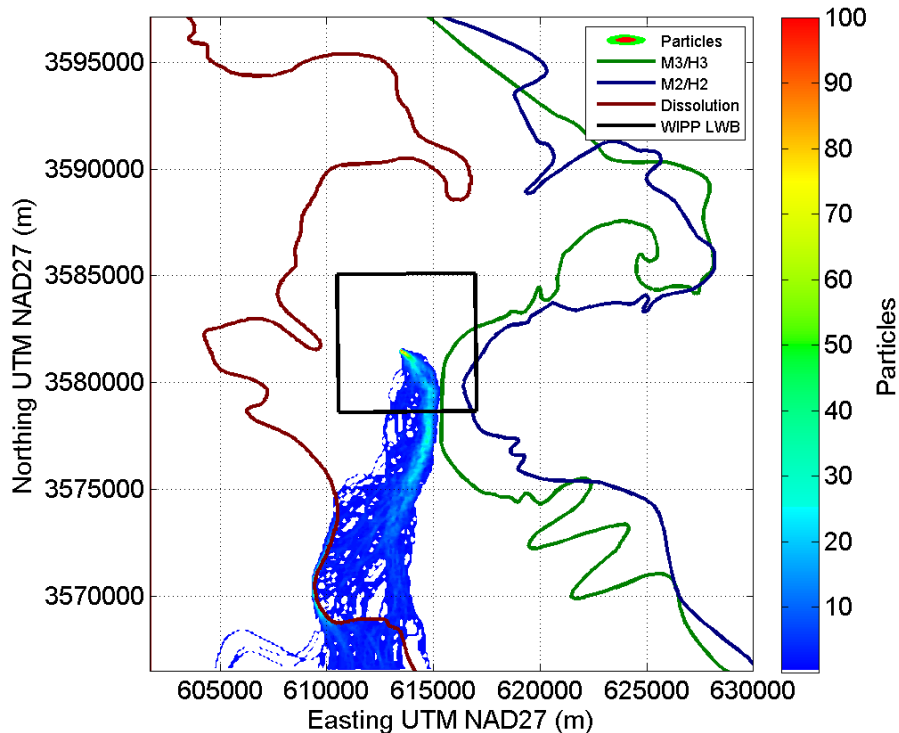The effects of the high-T channel can be seen in the flow paths (Hart et al. 2009).

Figure 8-4.   Particle Density in Each Cell for the 100 Final Selected Fields

(Hart et al. 2009)

8.5   MODIFICATIONS OF T-FIELDS FOR MINING SCENARIOS

Radionuclide movement through the Culebra is a function of the groundwater flow-field and the transport properties of the radionuclide species being considered. Groundwater flow velocity and direction are highly dependent upon the magnitude and the spatial variability of hydraulic transmissivity (the T-field). WIPP PA considers the potential that future potash mining in the McNutt potash zone of the Salado Formation underlying the Rustler Formation will cause subsidence in the Culebra and hence increase Culebra transmissivity.

The Culebra flow and transport begins with results from Latin Hypercube Sampling (LHS) (Kirchner 2010b) and the calibrated Culebra T-fields (Hart et al. 2009). Cumulative releases of radionuclides through the Culebra to the accessible environment (i.e., the Culebra outside the WIPP land withdrawal boundary) are inputs to CCDFGF (Camphouse 2010a). Discussion of the data flow between the different elements of PA can be found in the PABC-2009 summary report (Clayton et al. 2010).

The PABC-2009 Culebra T-field mining modifications and flow-field calculations performed by DOE largely follow the procedures used in the PABC-2004 (Lowry and Kanney 2005), with two exceptions: (1) a new definition of the region containing minable potash is used, and (2) the new T-fields developed and calibrated in Hart et al. (2009) are used as inputs. The procedures for DOE's analysis are summarized below:

(1) Obtain the sampled values for the random mining modification factor (100 vectors × 3 replicates)

(2) Map potential areas of future potash mining onto the groundwater modeling domain for both full- and partial-mining scenarios

(3) Apply the mining modification factor to the 100 stochastically calibrated T-fields from Hart et al. (2009), producing 600 mining-modified T-fields (100 vectors × 2 mining scenarios × 3 replicates)

(4) Perform steady-state flow simulations for each of the 600 mining-modified T-fields using MODFLOW-2000 (also known as MODFLOW or MF2K)

(5) Perform particle tracking using the new mining-affected flow-fields to determine advective travel times to the LWB

(6) Refine the flow-field to a finer grid size and re-execute MODFLOW to create flow-fields as input for the Culebra radionuclide transport calculations

Kuhlman (2010) details DOE's latest efforts in characterizing mining effects in the Culebra and highlights the differences and additions relative to past calculations (Ramsey et al. 1996; Lowry 2003a; Lowry 2003b; Lowry 2004).

The PABC-2009 models two categories of mining-impacted transmissivity fields; partial mining with only mining outside the LWB, and full mining with regions both inside and outside the LWB mined. Starting with the 100 stochastically calibrated T-fields from Hart et al. (2009), T-fields are modified to reflect the effects of mining by multiplying the transmissivity value in cells that lie within designated mining zones by a random factor uniformly sampled between 1 and 1,000. The range of this factor is set by the Agency in 40 CFR § 194.32(b) (EPA 1998e). The scaling factor for each T-field is provided from Latin Hypercube Sampling (LHS), (Kirchner 2010b).

DOE runs a forward steady-state flow simulation for each new T-field under each mining scenario (full and partial) across three replicates of mining factors, resulting in 600 simulations. Particle tracking is performed on both the 100 original and 600 modified flow-fields to compare the flow path and groundwater travel time from a point above the center of the WIPP disposal panels to the LWB. CDFs are produced for each mining scenario and compared to the undisturbed scenario. The CDFs describe the probability of a conservative tracer (i.e., a "marked" water particle) reaching the LWB at a given time. In addition to comparing travel times, particle-tracking directions are also examined to determine the effect on the regional flow direction in the WIPP area due to mining.

The parameter fields for the mining scenarios are then copied to a finer grid and the resulting flow-fields are passed to the transport analysis, which performs radionuclide transport modeling in the Culebra.

DOE's PABC-2009 analysis largely represents a re-application of the methods used in PABC-2004 (Lowry and Kanney 2005), with a few minor exceptions:

(1) The definition of the regions where minable potash is believed to exist, obtained from the Bureau of Land Management (BLM) (Cranston 2009), has been updated.

(2) The configuration of the MODFLOW model to which mining modifications are being applied has changed:

    a. The eastern limit of the model domain has moved 6 km east

    b. The no-flow boundary condition present along the western edge of the PABC-2004 model has been eliminated in the southern half of the model domain

    c. The "halite-sandwiched" region of the Culebra (east of either of the Rustler halite margins) is now constant head

(3) The way the mining-modified areas interact with internal boundary conditions of the flow model has changed, due to the change in the boundary conditions (there were no internal boundary conditions in the PABC-2004 MODFLOW model).

The PABC-2009 modeling domain and mining zones for the full-mining case are shown in comparison to the 1996 CCA and the CRA-2004 delineations in Figure 8-5. The comparison of the current and previous partial-mining cases is shown in Figure 8-6. A close-up of the WIPP site and the distribution of minable potash is shown in Figure 8-7 illustrating how the definition inside the WIPP LWB has changed significantly since the PABC-2004. For the PABC-2004, the closest minable potash was approximately 1,230 m from the center of the WIPP panels in the southeast direction; for PABC-2009, this distance has reduced to approximately 670 m (in a more easterly direction).

Compared to the non-mining scenario (Figure 8-2), the travel times for the partial-mining scenarios are longer, while travel times for the full-mining scenarios are shorter (Figure 8-8). The median travel time across all three replicates for the full-mining scenario is approximately 0.689 times the median travel time of the non-mining scenario. All advective particle travel times are plotted, but it should be noted that the regulatory limit for radionuclide transport modeling is 10,000 years, taking into consideration retardation, diffusion, and dispersion (which do not apply to particle track modeling). The median travel time across all three replicates for the partial-mining scenario is 3.034 times greater than for the non-mining scenario. For the partial-mining scenario, the increase in transmissivity due to mining increases the relative flow rate through the mining zones, with a corresponding decrease in flow through the non-mining zones. This decrease in flow through the non-mining zones produces longer travel times for the partial-mining scenario. For PABC-2004, travel times in both the full- and partial-mining scenarios were slower (longer) than for the non-mining scenario. The CDFs for the full-, partial-, and non-mining scenarios are shown in Figure 8-8.
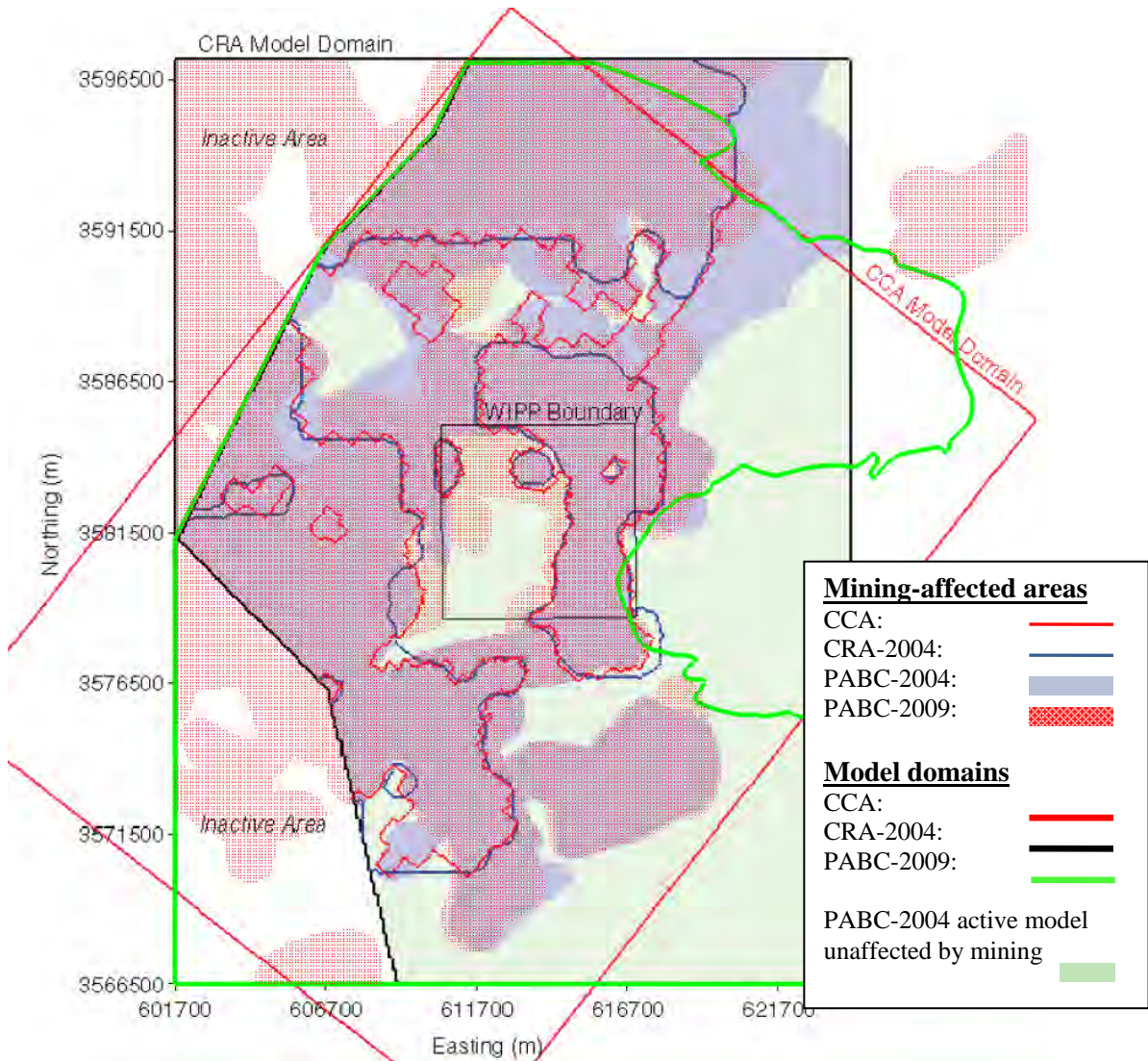
.

Figure 8-5.   Definitions of Mining-Affected Areas in Full-Mining Scenario between Current and Previous Models
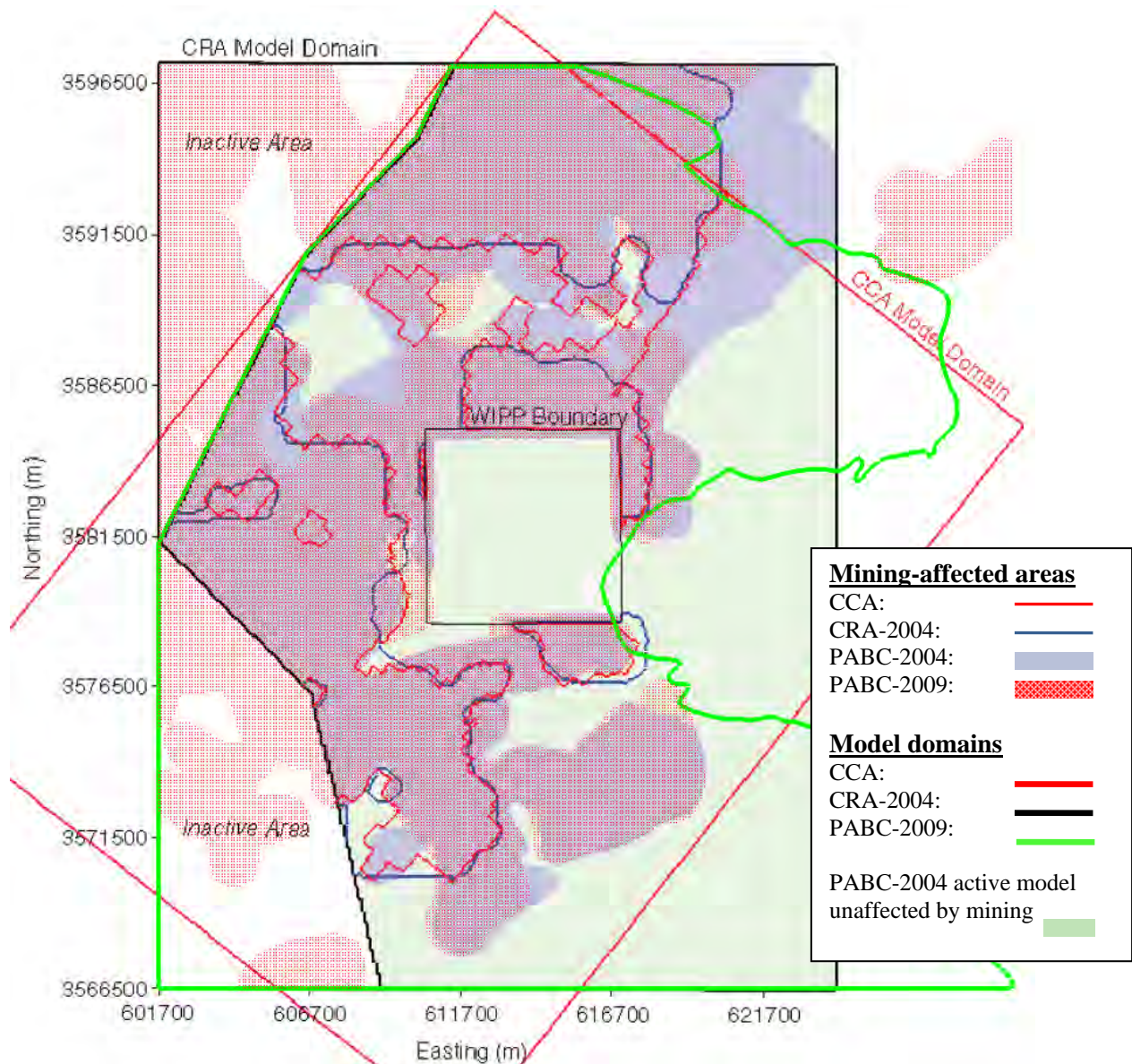
(Kuhlman 2010)

Figure 8-6. **Definitions of Partial-Mining-Affected Areas between Current and Previous Applications**
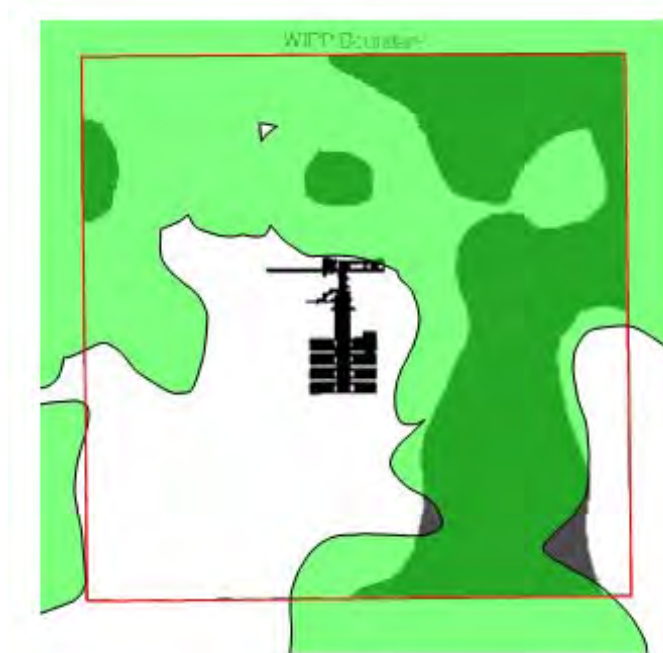
(Kuhlman 2010)

Figure 8-7. Comparison of Minable Potash Distribution Inside WIPP LWB for PABC-2004 (Dark Gray) and PABC-2009 (Transluscent Green)
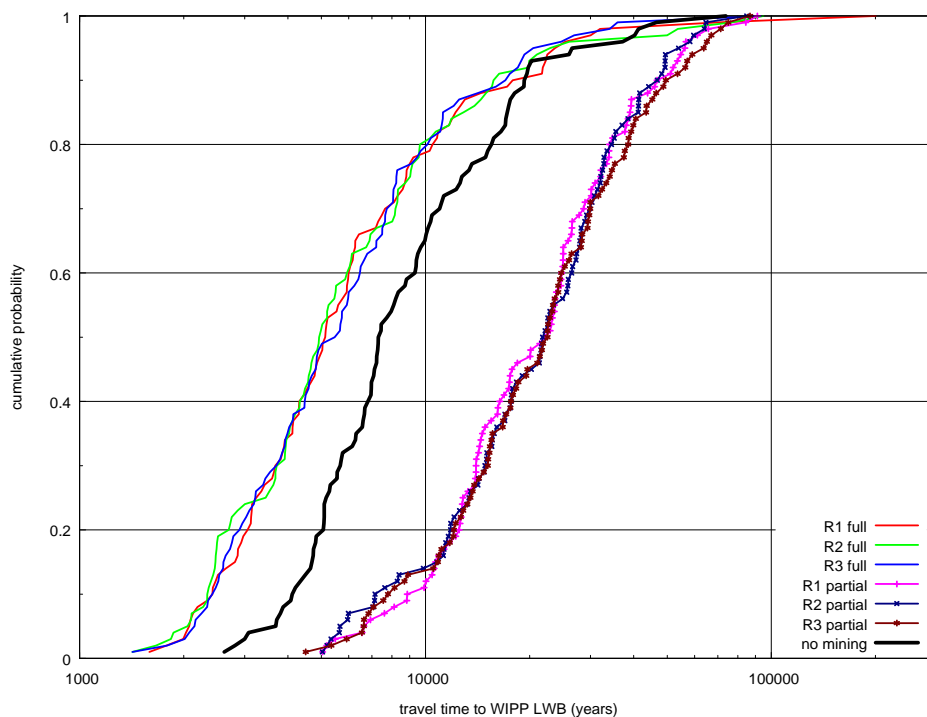
(Kuhlman 2010)

Figure 8-8. CDF of Advective Particle Travel Times from the Center of the WIPP Waste Panels to the WIPP LWB for Full, Partial, and Non-Mining Scenarios

(Kuhlman 2010)

9.0   CULEBRA DOLOMITE DISTRIBUTION COEFFICIENTS

Radionuclides may reach the Culebra member of the Rustler Formation via brine flow through a borehole that intersects the repository (DOE 2004b, Section 6.4.6.2.1; DOE 2009, Appendix PA, Section 6.8.3). Radionuclides introduced into the Culebra may then be transported by natural groundwater flow to the accessible environment (DOE 2004b, Section 6.4.6.2). Predictions of transport and release of radionuclides through the Culebra are affected by sorption onto minerals along this potential pathway. Accordingly, DOE developed distribution coefficients (K_ds) to express a linear relationship between sorbed and aqueous concentrations of the radionuclides (DOE 2004b, Section 6.4.6.2.1).

The distribution coefficients used in the CCA PA and PAVT were developed using data from experiments carried out at LANL and SNL (Table 9-1). EPA (1998d) evaluated the ranges and distributions of K_d values used in the CCA PA. EPA accepted the ranges, but disagreed with the uniform distribution for these ranges. EPA instead specified use of a log-uniform distribution for the K_d ranges in the CCA PAVT.

Table 9-1.   Comparison of Matrix K_d Values for the CCA PA and PAVT With Matrix Kd Values for the CRA-2004 PA, PABC04, CRA-2009 PA and PABC09

K_d Range [m³/kg]	CCA PA and PAVT (Brush 1996)	CRA-2004 PA, PABC04 and CRA-2009 PA (Brush and Storz 1996)	High Concentration Organics (Brush and Storz 1996)[a]	PABC09 (Clayton 2009b)[b]
Americium(III)	0.02–0.5	0.02–0.4	0.00505–0.00740	0.005–0.4
Plutonium(III)	0.02–0.5	0.02–0.4	--	0.005–0.4
Thorium(IV)	0.9–20	0.7–10	0.000467–0.00469	0.0005–10
Uranium(IV)	0.9–20	0.7–10	--	0.0005–10
Neptunium(IV)	0.9–20	0.7–10	--	0.0005–10
Plutonium(IV)	0.9–20	0.7–10	--	0.0005–10
Neptunium(V)	0.001–0.2	0.001–0.2	0.00–0.00249	0.00003–0.2
Uranium(VI)	0.00003–0.03	0.00003–0.02	0.00–0.0101	0.00003–0.02

a –   SPC brine (Salado) with 0.0489 M acetate, 0.003417 M citrate, 1.1×10^{-5} M EDTA, and 0.00288 M lactate; H-17 brine (Culebra) and ERDA-6 brine (Castile) with 0.0195 M acetate, 0.00340 M citrate, 1.46×10^{-5} M EDTA, and 0.00076 M lactate

b –   Log-uniform distribution

Brush and Storz (1996) revised the K_d values used in the CCA PAVT because of slight errors in the calculated K_d values. The differences between the K_d values reported by Brush (1996) and by Brush and Storz (1996) resulted from corrections of errors in the mass of dolomite used to calculate K_d values in one sorption study, and corrections of errors in the density of brine used to calculate K_d values in another set of experiments (Brush and Storz 1996). The revised values from Brush and Storz (1996) were not available in time for inclusion in the CCA PA or PAVT; however, Brush and Storz (1996) stated that the relatively small changes in the K_d values were unlikely to significantly impact PA results. The corrected K_d values (Brush and Storz 1996) were used in the CRA-2004 PA and PABC04. EPA (2006d) determined that the revised K_d ranges used in the CRA-2004 PA and PABC04 were acceptable, because no new experimental sorption data were available, the changes to the K_d ranges were minor and conservative, and these changes had been previously reviewed and found acceptable by EPA (1998d).

Experimental data regarding the potential effects of organic ligands on actinide sorption were considered by EPA (1998d). At that time, EPA concluded that the results of the speciation calculations, K_d values reported in the literature and expected increased adsorption under alkaline conditions indicated that the K_d ranges exclusive of the organic ligands were sufficiently representative of actinide solid/liquid partitioning for modeling actinide transport in the Culebra. However, aqueous speciation data and modeling calculations available from the CRA-2004 (EPA 2006d, Section 8.0) indicated that solubilities of the +III and +V actinides could be affected by organic ligands. Consequently, EPA (2006d) re-examined the K_d values measured in brines with organic ligands (Brush and Storz 1996). The reported values for low and intermediate organic ligand concentrations were judged to be the most applicable to WIPP repository conditions. EPA (2006d) concluded that the range of K_d values used for the CRA-2004 PA and PABC04 (Brush and Storz 1996) were acceptable, because no new experimental sorption data were available, the changes to the K_d ranges were minor and conservative, these changes had been previously reviewed and found acceptable by EPA (1998d), and relatively low concentrations of organic ligands would not significantly affect the K_d ranges.

Higher organic ligand concentrations have been predicted for the PABC09 than for previous PAs (Table 7-2). The current predicted acetate and citrate concentrations are similar to concentrations in the high-ligand-concentration experiments reported by Brush and Storz (1996), and the current predicted EDTA concentration exceeds the concentrations reported for the high-ligand-concentration experiments. EPA requested additional information from DOE regarding the possible effects of increased ligand concentrations and lower K_d values on +III and +IV actinide releases by transport through the Culebra (Comment 3-C-25, Cotsworth 2009c).

DOE re-evaluated the range of K_d values used to assess retardation of actinides during transport through the Culebra (Moody 2010b). There was no evidence indicating that the upper bound should be changed. Consequently, the upper bounds for the K_d ranges were maintained, but the lower bounds were reduced to account for the possibility of higher organic ligand concentrations.

Clayton (2009b) provided details regarding the changes in the K_d ranges. The lower limit for the uranium(VI) K_d range was not modified, because this value was already effectively equal to zero. Although neptunium is not currently included in the Culebra transport calculations, DOE updated its K_d range to maintain consistency. Because the K_d ranges sampled for PA are assumed to have a log-uniform distribution, assumption of a lower K_d limit of zero is not valid. Consequently, the lower limit of the uranium(VI) K_d was also assumed for the lower limit for the neptunium(V) K_d. The K_d ranges used in the PABC09 are summarized in Table 9-1. The revised lower-bound values for the K_ds used in the PABC09 are consistent with the lower limits of the ranges observed in the experiments with high concentrations of organic ligands. Consequently, EPA (2010e) determined that the K_d ranges were appropriate for use in the PABC09.

10.0   SALADO FLOW AND TRANSPORT

10.1   INTRODUCTION

The WIPP PA consists of a suite of software designed to predict conditions in and around the repository over a period of 10,000 years. One of the first models that is run for PA is the BRAGFLO software (Nemer 2007a and 2007b), which simulates brine and gas flow in and around the repository. BRAGFLO includes the effects of processes such as gas generation and creep closure. Outputs from the BRAGFLO simulations describe the conditions (pressure, brine saturation, porosity) and flow patterns (brine flow up an intrusion borehole and out anhydrite marker beds to the accessible environment) that are used by other software to predict radionuclide releases.

The CRA-2009 PA was run under AP-137, *Analysis Plan for the Performance Assessment for the 2009 Compliance Recertification Application, Revision 1* (Clayton 2008). An analysis report was written (Nemer and Clayton 2008) summarizing the BRAGFLO results. Changes in the CRA-2009 BRAGFLO analysis from the PABC-2004 BRAGFLO analysis included:

(1) Additional CPR inventory due to the emplacement materials
(2) Slightly higher halite and DRZ porosity
(3) Slight modification to the way in which the humid CPR degradation rate is calculated
(4) Change to the way in which the effective saturation is calculated at low saturations
(5) Additional smoothing to chemical reaction rates
(6) New capillary-pressure model for open cavities

EPA required that the DOE revise the CRA-2009 analysis and present the new results before the the Agency would judge the CRA-2009 to be complete (Cotsworth 2009a). The EPA noted a number of technical changes and corrections to the CRA-2009 PA that it deemed necessary. The only change mandated by the EPA that affects the BRAGFLO portion of WIPP PA is an updated inventory. For the PABC-2009 BRAGFLO calculations, inventory from the Performance Assessment Inventory Report (PAIR) – 2008 (Crawford et al. 2009) was used. The Agency has reviewed the changes implemented in the PABC-2009 and has determined that they satisfy the concerns raised by the Agency.

Between the CRA-2009 and the PABC-2009 analysis, there are two sets of parameter changes that have a significant impact on Salado transport. The CRA-2009 PA used the inventory from the CRA-2004 PABC; this has since been updated, and the most recent inventory report has been used (Fox et al. 2009). Among the changes to the inventory was a redistribution in the relative amounts of different isotopes in the repository, which will lead to changes in potential releases as a result of the different half-lives of different waste components. The net increase in the total inventory of the repository that contributes to the Waste Unit Factor (WUF), from 2.32 MCi to 2.6 MCi, is not expected to cause a significant change in behavior, as the definition of EPA units for releases takes the total inventory of the repository into account. In a separate change, the probability distribution for the baseline solubility limit for +III and +IV actinides has been revised (Brush et al. 2009; Xiong et al. 2009). The new distributions for the solubility limits change the amount of actinides that can be dissolved into any brine that may be present, and

consequently the amount of actinides that can reach the surface or the Land Withdrawal Boundary (LWB). As discussed in Section 3, EPA has determined that the inventory documented in the PAIR 2008 is appropriate for use in PA.

10.2   MODELING SCENARIOS

For transport of radionuclides within the Salado Formation, the presence of brine is required. There are two main sources of brine available within the repository. First, a limited quantity of brine is contained in inclusions in the rock surrounding the WIPP repository. WIPP PA assumes that all of the brine in the Disturbed Rock Zone (DRZ) will be available for reaction with the waste in the repository. Additionally, in the case of an intrusion into and below the repository that penetrates a brine pocket in the Castile Formation underneath the repository, substantial quantities of brine may flow into a panel. However, because the location of brine pockets underneath the repository is unknown, it is not guaranteed that an intrusion through the repository will intersect a brine pocket.

There are two primary mechanisms by which radionuclide-contaminated brine can reach the WIPP boundary via flow and transport mechanisms. Brine in the repository can flow through the Salado marker beds towards the Land Withdrawal Boundary (LWB). In addition, following an intrusion, brine can flow up the resulting borehole until it comes into contact with the Culebra Dolomite member of the Rustler Formation. The upflowing brine is added to that in the Culebra, which is then transported laterally towards the LWB.

To represent possible future states of the repository and to predict possible releases through the Salado and to the Culebra, WIPP PA considers six different modeling scenarios, that are differentiated by the number of intrusions, the time at which intrusions occur and whether or not the intrusion encounters a brine pocket.

The first five scenarios are modeled using NUTS (Section 10.6), while the sixth scenario is modeled using PANEL. Scenario 6 cannot be modeled in NUTS because the model for the two-intrusion scenario assumes that the two boreholes are drilled in different locations; this assumption cannot be explicitly handled in NUTS unless it is first modeled in BRAGFLO or another fluid transport code, as NUTS does not compute its own flow fields.

10.3   POTENTIAL RELEASE SCENARIOS

Nemer (2010) gives a complete analysis of the Salado flow results. When brine enters the disposal region, gas is generated by anoxic corrosion of iron and biodegradation of organic materials. Corrosion of the metal containers, along with structural deformation caused by the viscoelastic response of the mined salt, leads to container failure and the eventual release of radioisotopes into the brine from the waste. If sufficient quantities of gas are generated, pressures in the disposal region will increase, reducing brine flow into the repository. Brine containing dissolved radioisotopes may be expelled from the repository if pressure in the repository exceeds the brine pressure in the immediately surrounding formation. In addition, brine saturation in the waste must exceed residual brine saturation in order for brine to be expelled from the repository.

Three potential pathways for migration of radioisotopes in dissolved brine are considered in this analysis. The first and most important pathway is a human intrusion into and possibly through the repository. Under this scenario, brine may be released up the borehole toward the Culebra Dolomite member of the Rustler formation. Once in the Culebra, contaminated brine may then move toward the subsurface land withdrawal boundary. Direct brine releases to the surface are modeled and analyzed using a different code, and are considered in Section 11.2. In the second pathway, brine may migrate through or around the panel seals through the DRZ surrounding the repository to the shaft and then upward toward the Culebra. In the third pathway, brine may migrate from the repository through the DRZ and within the anhydrite interbeds (Marker Beds 138 and 139) laterally toward the subsurface land withdrawal boundary.

The dynamics of brine movement are complex and highly dependent on the Salado flow input parameters. Initially, brine may flow into the repository from any one of the migration pathways mentioned above. If sufficient brine enters the repository the radioisotopes become mobilized in both solute and colloidal sorbed forms. Once the radioisotopes are mobilized, transport away from the repository can only occur if the head potential within the repository exceeds that outside the repository and if brine saturation in the waste exceeds residual brine saturation.

10.4   GENERAL MODELING APPROACH

Flow in the Salado is computed by BRAGFLO (Nemer and Clayton 2008), which simulates brine and gas flow in and around the repository. BRAGFLO includes the effects of processes such as gas generation and creep closure. Outputs from the BRAGFLO simulations describe the conditions (pressure, brine saturation, porosity) and flow patterns (e.g., brine flow up an intrusion borehole and out anhydrite marker beds to the accessible environment) that are used by other software to predict radionuclide releases. Some of the specific processes included in the BRAGFLO calculations include:

- Brine and gas flow

- Creep closure of the waste-filled regions within the repository

- Gas generation due to corrosion of steel and decomposition of biodegradable materials (cellulosics, plastics, and rubbers)

- Physical changes (e.g. permeability and porosity) in the modeling domain over time

- Consequences of rock fracturing due to high pressure

The overall transport and decay of radionuclides in the Salado is calculated using the computer code NUTS (NUclide Transport System). NUTS is a five-point finite difference code designed to model multi-dimensional, multi-component and radioactive-contaminant transport in single-porosity, dual-porosity and/or dual-permeability porous media, including parent/daughter first-order decay. The key processes modeled with NUTS are advective transport, decay, precipitation, solubility limits and interior sources, all in a continuous matrix. No dispersion is modeled. The initial condition for each run is to assume no contamination present within the model domain, with the exception of the source term in the waste panel area.

Any flow of brine up the shafts, borehole(s) and out the marker beds is calculated using BRAGFLO, and these results are required prior to running NUTS. This input is an ASCII file containing the grid specifications, initialization parameters and material maps as well as the BRAGFLO post-processed binary file (CDB) that describes the flow-field. The CDB files are the source for brine fluxes at the cell interfaces, porosity, saturation, pressure and the geometric information. In addition, NUTS uses a CDB file that contains the "effective solubilities," "lumped inventory" source terms created by PANEL (Garner and Leigh 2005), and atomic weights and half-lives of the modeled isotopes. NUTS also uses its own input files that contain the run parameters and the isotope decay data.

The mathematical formulations and model conceptualizations of both BRAGFLO and NUTS have been evaluated by EPA and found to be acceptable (EPA 1998b).

In the CRA-2009 and PABC-2009, the same disposal system geometry was used in both the BRAGFLO and NUTs computational models. Four different maps of material properties were assigned: one for undisturbed conditions; one for the E1 intrusion event, in which a borehole penetrates the panel and a Castile brine reservoir; one for the E2 intrusion event, in which a borehole penetrates the repository but not a Castile brine reservoir; and one for the E1E2 intrusion event, in which at least one E1 borehole and one other borehole penetrate a disposal panel. The geometry and material maps used for each scenario were similar. Each is a model for fluid flow and radionuclide transport calculations that represents the three-dimensional physical system in a two-dimensional plane that cuts vertically through the repository and surrounding strata. Side views of the vertical cross section and two of the material maps used in CRA-2009/CRA-2009PABC are presented in Figures 10-1 and 10-2 (Nemer and Clayton 2008).

10.5   SALADO FLOW ANALYSIS

The conceptual models implemented in the BRAGFLO simulations for the PABC-2009 are unchanged from those used in the CRA-2009 PA.

10.5.1 SANTOS

Several steps must be completed before the BRAGFLO analysis can begin. Creep closure calculations (SANTOS) must be available and an ASCII input file created that contains information about the porosity surface(s) to be used in the BRAGFLO calculation. The ASCII file used for the PABC-2009 is identical to those used for the PAVT and CRA-2009 calculations.

In 2005, the Agency reviewed SANTOS and concluded that although the accuracy of the SANTOS calculations may be limited, the SANTOS model is capable of reproducing the fundamental aspects of the conceptual model including simulation of the large-scale halite deformation and waste compaction accompanying room closure (EPA 2005b). EPA further concluded that the approximations of room closure and waste compaction developed by the SANTOS model are adequate for use in WIPP PA.

10.5.2 BRAGFLO

10.5.2.1   Model Geometry

The BRAGFLO grid used for PABC-2009 BRAGFLO calculations is the same as that used for the CRA-2009 PA (Nemer and Clayton 2008). This grid is shown as a logical grid with dimensions in Figure 10-1 and it is shown from the top, displaying its radial flaring in Figure 10-2.

The primary objective in creating the modeling grid for BRAGFLO is to capture the effects of known and significant hydrologic features in and around the repository. This is accomplished by using a vertical, two-dimensional grid, oriented south to north through the repository and surrounding strata (Figure 10-2). The lengths (Δx), the widths (Δz), and the heights (Δy) of each grid cell are indicated in Figure 10-1. The wide variation in grid cell dimensions captures a relatively large amount of detail with a relatively small number of grid cells.

The two-dimensional BRAGFLO grid captures three-dimensional flow effects by employing the technique of "radial flaring." This flaring is visible when looking down on the grid from the top, as shown in Figure 10-2. In this figure, the width of each grid cell to the north and south of the repository increases with distance away from the center of the waste-filled region. The flaring simulates convergent or divergent flow to the north and south centered on the repository, and laterally away from the repository. The flaring methodology used to create the grid is discussed in a separate memorandum (Stein 2002). This general methodology was tested in WIPP PA (SNL 1996) and shown to adequately represent fluid releases when compared to an alternative three dimensional approach, which is more computationally expensive.

The Salado flow grid incorporates the repository, the Castile brine reservoir, the Salado Formation, bedded units above the Salado, the shaft, panel seals and an intrusion borehole used for disturbed scenarios. The analysis report for CRA-2004 (Stein and Zelinski 2003) provides a detailed explanation of all the stratagraphic and other materials used to represent the repository and surrounding units.
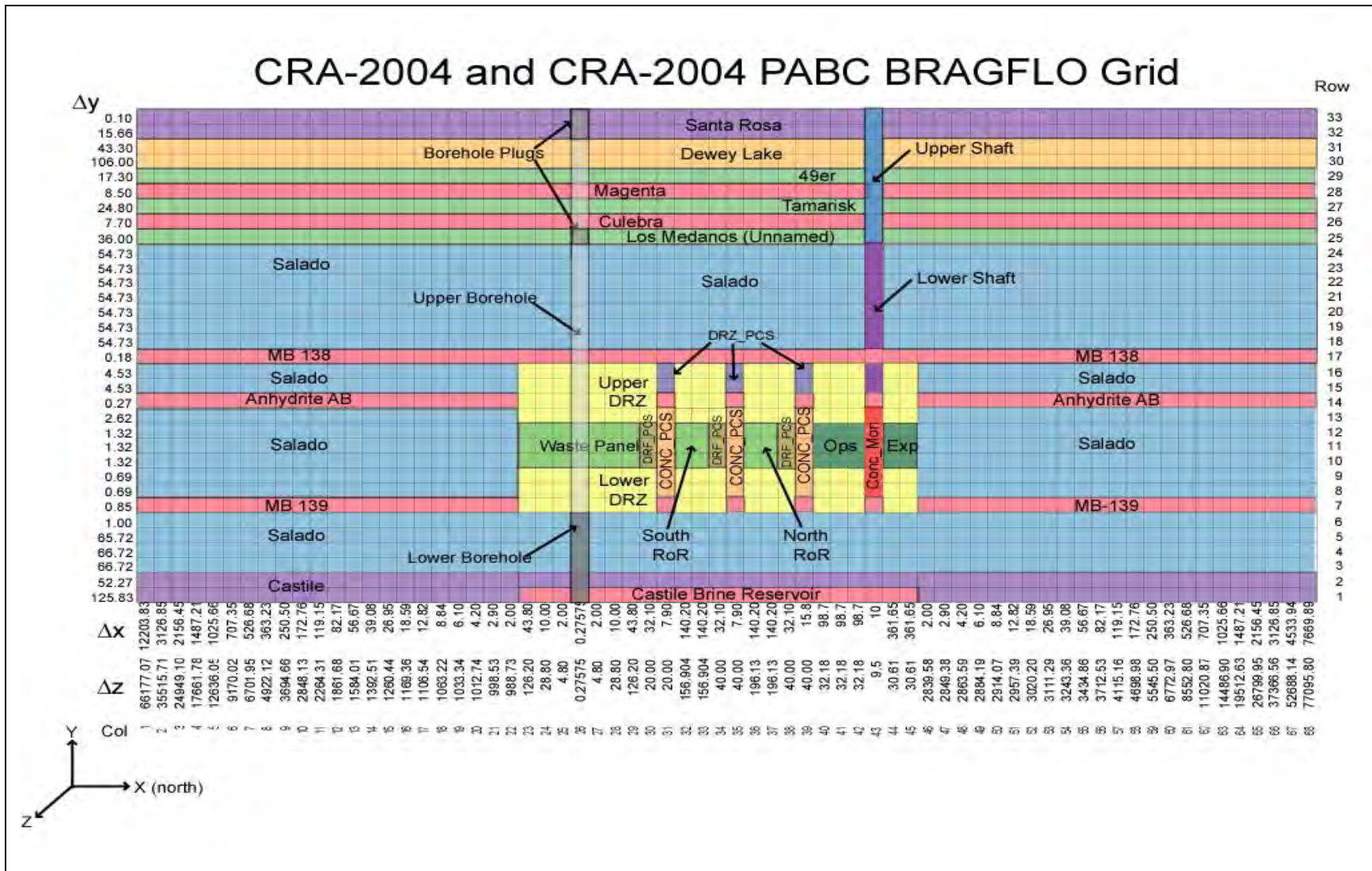
Figure 10-1. PABC-2009 BRAGFLO Grid (Δx, Δy, and Δz dimensions in meters)

Note that "north of the repository" is to the right of the Exp area on the above graph and "south of the repository" is to the left of the Panel area.
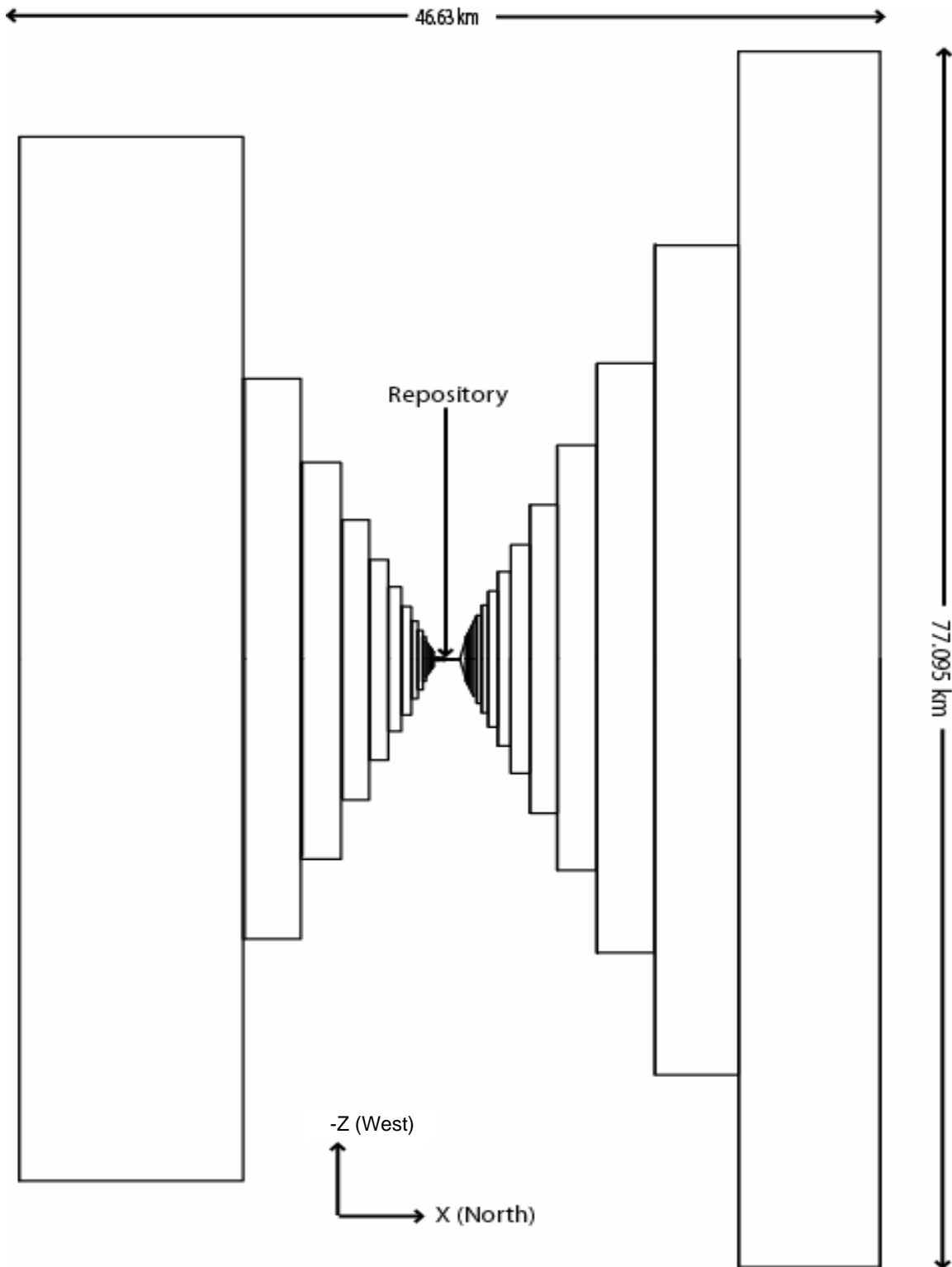
Figure 10-2. Top View of PABC-2009 Logical Grid showing the Radial Flaring

10.5.2.2   Initial and Boundary Conditions

BRAGFLO simulation of brine and gas flow in the vicinity of the WIPP site requires the assignment of initial and boundary conditions including brine pressure, brine saturation, and concentrations of iron and biodegradable material. These initial conditions are provided to BRAGFLO through various pre-processing steps during which values are extracted or sampled from the WIPP PA Performance Assessment Parameter Database (WIPP PAPDB).

At the beginning of each BRAGFLO run (scenario-vector combination), the model simulates a short period of time representing disposal operations. This portion of the run is called the initialization period and lasts for 5 years (from t = -5 to 0 years), corresponding to the time a typical waste panel is expected to be open during disposal operations. All grid blocks require initial pressure and saturation at the beginning of the run (t = -5 years). At the beginning of the regulatory period (0 to 10,000 years), BRAGFLO resets initial conditions within the excavated regions and in the shaft.

During the initialization period, brine tends to flow into the excavated areas and the shaft, resulting in decreased pressure and saturation in the rock immediately adjacent to the excavations. At time t = 0, the pressure and saturation in all the excavations are reset to initial conditions for the materials used to represent these regions for the regulatory period. This practice is intended to capture the effect of evaporation of brine inflow during the operational period and the transport of this brine up the shaft ventilation system, as well as the depressurization of the surrounding rock formations due to excavation.

BRAGFLO simulation of brine and gas flow in the vicinity of the WIPP site requires the assignment of initial conditions including brine pressure, brine saturation and concentrations of iron and biodegradable material. These initial conditions are provided to BRAGFLO through various pre-processing steps during which values are extracted or sampled from the WIPP PA Parameter Database.

The boundary conditions assigned for the BRAGFLO calculations in the PABC-2009 are the same as the CRA-2009 PA:

- Constant pressure at the north and south ends of the Culebra and Magenta Dolomites.

- Constant pressure (1.01325×10^5 Pa) and saturation (0.08363 dimensionless) (Vaughn 1996) conditions at the land surface boundary of the grid, except at the shaft cell on the land surface boundary. The saturation constraint has been removed from the shaft cell that lies at the land surface because at t = 0, the saturation in this cell is reset along with the rest of the shaft to the initial saturation in the WIPP parameter database (SAT_IBRN) for each of the respective shaft materials. The combination of a fixed saturation boundary condition equal to 0.08363 and simultaneously being reset at t = 0 to 0.796 (SHFTU:SAT_IBRN) had the potential to create numerical difficulties.

- No flow conditions at all other grid boundaries.

10.5.2.3   BRAGFLO Predictions

The brine release volume is the dominant variable associated with predicting releases. Consequently, DOE has plotted the brine release volumes for the PABC-2009 versus the corresponding CRA-2009 brine release volumes in Figure 10-3. As shown in Figure 10-3, the brine volumes are essentially equal, and particularly for releases of 10 m^3 or more; discrepancies between the predictions are typically decreases in volume from the CRA-2009 to the PABC-2009. As a result, it would be expected that there would be roughly comparable releases for the CRA-2009 and PABC-2009, with deviations between the two being the result of the minor changes to the input parameters—solubility limits and inventory—provided to PANEL.
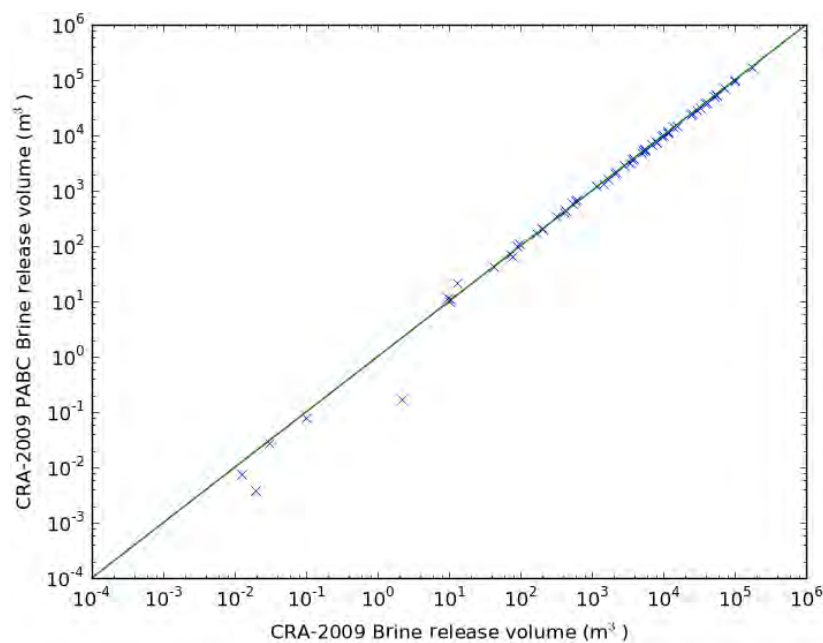

Figure 10-3.   PABC-2009 versus CRA-2009 Release Volumes for Replicate 1, Scenario 6

10.5.3 Salado Flow Summary and Conclusions

The BRAGFLO analysis provides essential outputs that are needed by other PA process models in order to calculate total releases from the repository. Results of the CRA-2009 PA and the PABC-2004 were compared. For the S1 scenario, pressures and saturations in the CRA-2009 PA and the PABC-2004 were similar at 10,000 years. Brine flows into the repository were generally greater in the CRA-2009 PA than the PABC-2004 due to the higher DRZ porosities.

Microbial gas generation was slightly higher in the CRA-2009 PA than the PABC-2004, owing to the addition of the emplacement materials and the increased DRZ porosity. The new methodology for sampling the humid rate had a modest effect on microbial gas generation, which is as intended.

The changes to the BRAGFLO code had little effect on the results other than to cause fewer exception vectors when the repository becomes dry. Because these vectors are generally at lower pressures and saturations, their effect is minimal on repository performance.

In the CRA-2009 PA fracture lengths were generally higher than in the PABC-2004; however, this result should be considered with the caveat that the pressures generating these larger fracture lengths were only slightly different than that of the PABC-2004. DOE notes that the larger fracture length did not lead to a significantly larger brine release to the LWB.

The results from the PABC-2009 BRAGFLO calculations were nearly identical to those of the CRA-2009 PA. A slightly lower inventory of CPR and iron caused slightly lower pressures in the repository. Lower pressures caused less fracturing of the marker beds.

Based upon the Agency's review of the modifications to the BRAFLO flow modeling in conjunction with the fact that the BRAGFLO results from the PABC-2004 are very similar to those obtained from the PABC-2009, the Agency accepts the BRAGFLO flow results for flow within the Salado.

10.6   SALADO TRANSPORT ANALYSIS

Radionuclide releases from the repository to the Culebra depend on the rate of brine flow, the solubility limits, and the amounts of radionuclide available for transport. Radionuclides are assumed to exist in five states that can be transported from the repository by flowing groundwater (Helton et al. 1998)—dissolved, humic colloids, microbial colloids, mineral fragment colloids and actinide intrinsic colloids. The concentration in each of these states is a function of one or more sampled variables. Effective solubility is defined to be the maximum concentration that the brine can hold including both radionuclides suspended on colloids and dissolved in the brine. Stockman et al. (1996) and Garner (2003) provide a full discussion on effective solubility related to the radionuclide transport calculations. Mobilization is assumed to be instantaneous at the solubility limit (or the inventory limit, whichever is lower) such that the radionuclide concentrations in the brine and on the colloids are always at equilibrium. However, since the isotope inventory changes with time as a result of decay and in-growth, steady-state equilibrium is not achieved.

For the transport analyses the overall transport and decay of radionuclides are calculated using NUTS, version 2.05c (EPA 2010c). NUTS is a multidimensional, multi-component radioactive material contaminant transport, single-porosity (SP), dual-porosity (DP), and dual-permeability (DPM) finite-difference simulator. The model simulates first order radioactive chain decay during radioactive material transport. The key processes modeled are advective transport, or transport caused by the velocity field of the fluid; decay of radionuclides; precipitation of radionuclides from solution; solubility limits controlling the amount of radionuclides permitted in the aqueous phase; and the existence of finite radionuclide sources anywhere in the interior of the computational grid. Dispersion, which smears the concentration profile in the direction of fluid flow, is not modeled (Treadway 1997). The initial condition for each run is to assume that, with the exception of the source term in the waste panel area, no radionuclides are present within the model domain.

As discussed previously, any flow of brine up the shafts or boreholes or through the marker beds is calculated using the code BRAGFLO, which must be run prior to running NUTS. NUTS uses multiple input files, including the BRAGFLO ASCII input file containing the grid specifications, initialization parameters, and material maps as well as the BRAGFLO post-processed binary file (CDB) that describes the flow field. These CDB files are the source for brine fluxes at the cell interfaces, porosity, saturation, pressure and the geometric information. In addition, NUTS uses a CDB file that contains "effective solubilities," and "lumped inventory" source terms created by PANEL, and atomic weights and half-lives of the modeled isotopes plus an input file specific to NUTS, containing run parameters and isotope decay data information. The BRAGFLO output CDB file is now processed using MATSET to add a number of parameters from the PA parameter database needed for analysis by ALGEBRA.

10.6.1 Salado Transport Results

In WIPP PA, three different types of runs are performed with NUTS: screening, which identifies those vectors which must be analyzed in greater detail; isotope, which determines the amount of radionuclides transported throughout the repository; and time-intrusion, which repeats the isotope calculations with different starting times.

The maximum and average releases obtained in the two analyses performed in the PABC-2009 and in the CRA-2009 calculations (Ismail and Garner 2008) are shown in Figure 10-4 and Figure 10-5, respectively. Examining the maximum releases, it is apparent that the maximum total releases in the PABC-2009 are uniformly larger than the corresponding cases from the CRA-2009 PA. However, the increases are relatively minor, and do not necessarily correspond to directly comparable circumstances, as different vectors are involved across the different analyses. Moreover, the increase in the maximum releases will not necessarily have a significant impact on repository performance, as they represent only releases to the Culebra; transport from the borehole to the LWB must also occur before they reach the accessible environment. DOE notes that the reason for the increases is the higher solubilities of dissolved actinides for the PABC-2009 versus the CRA-2009 (Xiong et al. 2009; Garner 2010).

Examining the average releases in the three analyses, there is much more consistent behavior across the different intrusion times considered. The differences between the average releases in the various analyses are much smaller than the difference in the maxima. Consequently, DOE asserts that the changes in "outlier" vectors do not have a significant impact on the average behavior of the system.

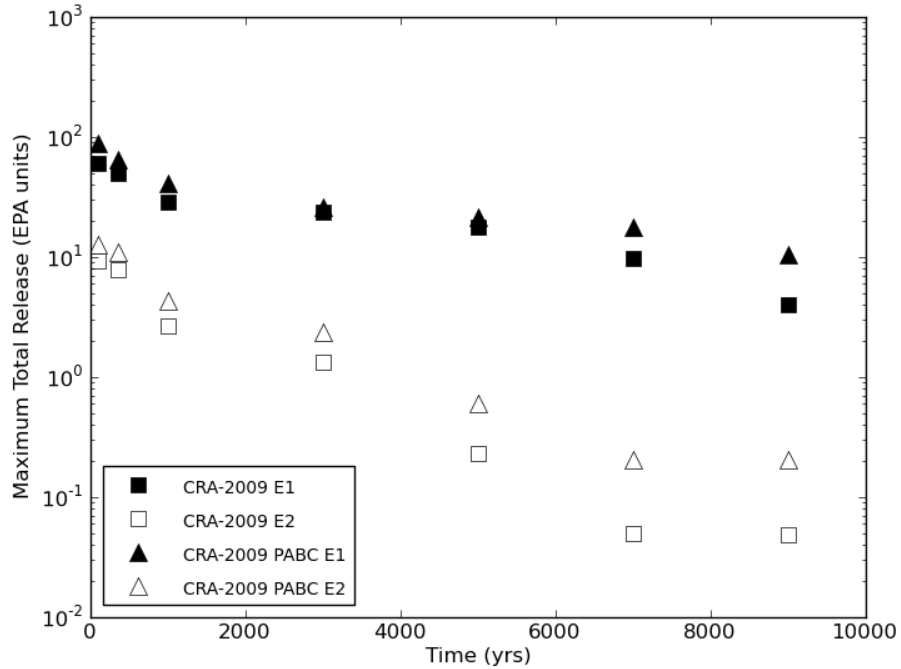**Figure 10-4.** **Maximum Releases (in EPA units) as a Function of Time and Intrusion Type for the CRA-2009 and PABC-2009**
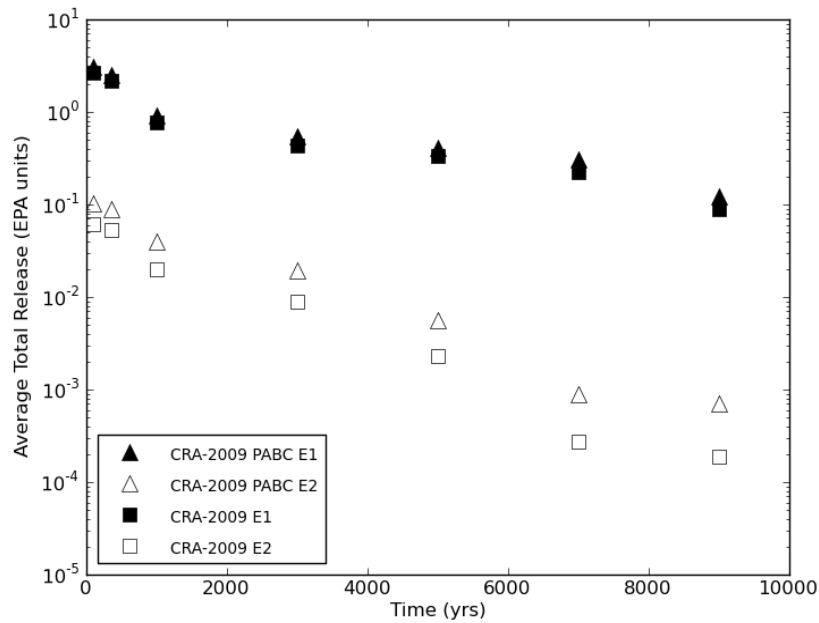

Figure 10-5. **Average Releases (in EPA units) as a Function of Time and Intrusion Type for the CRA-2009 and PABC-2009**

10.6.2 Salado Transport Summary and Conclusions

The calculations performed to support the PABC-2009 are based on the same process as the PABC-2004 (Garner and Leigh 2005; Lowry 2005) and the CRA-2009 (Ismail and Garner 2008). The primary changes affecting the results are the changes in the inventory and in the revised concentrations of dissolved actinides. The number of vectors with measurable releases is essentially identical, and releases are of comparable orders of magnitude, although releases are slightly larger in the PABC-2009. However, DOE states that these changes ultimately will have a negligible impact on repository performance, because material released to the Culebra from the Salado must first make its way through the Culebra before reaching the accessible environment outside the LWB.

Calculations from PANEL show only small differences in the results between the CRA-2009 PA and the PABC-2009. Release volumes were essentially unchanged between the two sets of calculations, and any changes were for release volumes less than about 10 m^3, which are not large enough to have a significant effect on overall releases.

11.0   DIRECT RELEASES

Direct releases are defined as solid and liquid materials removed from the repository and carried to the ground surface through intrusion boreholes at the time of drilling. Direct releases occur in WIPP PA through cuttings and cavings releases, direct brine releases (DBRs) and spallings releases. The Agency evaluated these release modes in their PABC-2009 assessment and compared them with releases projected in the PABC-2004.

11.1   CUTTINGS AND CAVINGS CALCULATIONS

Cuttings and cavings are the solid materials removed from the repository and carried to the ground surface by drilling fluid during the process of drilling a borehole that intersects the repository. Cuttings are the materials removed directly by the drill bit and cavings are the materials eroded from the borehole walls by shear stresses from the circulating drill fluid (Clayton et al. 2010, Section 3.6). The CUTTINGS_S code is used in WIPP PA to calculate cuttings and cavings release volumes. Inputs to the CUTTING_S code include drilling characteristics such as bit size, rotational velocity and drill fluid properties, as well as waste shear strength. The radiological properties of the cuttings and cavings release volumes are calculated by the CCDFGF code (Vugrin 2005a, Section 2.1).

11.1.1 Modifications since the PABC-2004

Although the CUTTINGS_S code has been revised a number of times since the Agency's original WIPP compliance certification, the fundamental cuttings and cavings calculation approach has not changed. CUTTINGS_S Version 5.04 was used in the PAVT. It was subsequently revised to Version 5.04A and then to Version 5.10 used in the CRA-2004 PA. Following the CRA-2004 PA, CUTTINGS_S was revised to Versions 6.00 and 6.01, and then to Version 6.02, which was used in the PABC-2004. The modifications made in each revision are summarized in EPA 2006c, Section 10.1.1. CUTTINGS_S Version 6.02 was also used in the CRA-2009 PA (Long 2008, Table 4.1) and in the PABC-2009 (Long 2010, Table 4.1). The Agency continues to consider the CUTTINGS_S code to be appropriate for use in WIPP PA. Validation of the CUTTINGS_S code is reviewed in EPA 2006e.

11.1.2 Calculation Results

The direct releases from cuttings and cavings as calculated for the PABC-2009 are presented in Ismail 2010, Section 4.1, and summarized in Clayton et al. 2010, Section 5.5.2. The CUTTINGS_S code calculates cuttings and cavings together. The volume of contact-handled (CH) cuttings and cavings material removed from a single drilling intrusion into the repository is assumed to be in the shape of a cylinder with a height equal to the initial repository height of 3.96 m. The CUTTINGS_S code calculates the area of the base of this cylinder, and cuttings and cavings results are reported in terms of this area. Cuttings and cavings areas calculated for the PABC-2009 range between 0.076 m^2 and 0.86 m^2 (Clayton et al. 2010, Table 5-3). These results are the same as calculated for the PABC-2004 (Leigh et al. 2005a, Table 5-4). All realizations had cuttings releases and about 90% of the realizations also had cavings releases (Clayton et al. 2010, Table 5-3). The corresponding release volumes ranged from 0.30 m^3 to 3.41 m^3 and

averaged about 1.0 m^3. The release volumes for remote-handled (RH) waste are somewhat less because of the smaller height of an RH waste canister (0.509 m) (Dunegan 2004).

Because cuttings releases occur with every borehole penetration, the combined cuttings and cavings release is lowest when no cavings occur. This minimum value is a function of only the drill bit diameter and the initial repository height, neither of which is treated as an uncertain parameter. Cuttings releases are therefore the same in every realization and have the relatively small release volume of 0.30 m^3. The cavings volumes generally account for the bulk of the combined cuttings and cavings releases and are affected by two uncertain parameters: the shear strength of the waste and the drill string angular velocity. Lower shear strengths and higher angular velocities result in greater cavings releases (Leigh et al. 2005a, Section 7.3). These results are reasonable and appropriate, and are similar to the results obtained in earlier PA analyses.

Figure 11-1 illustrates the differences between the normalized cuttings and cavings radionuclide releases for the PABC-2004 and PABC-2009, expressed as the combined mean complimentary cumulative distribution functions (CCDFs) for the three PA replicates. Comparison of these curves shows that the mean cuttings and cavings radionuclide releases remained essentially unchanged in the PABC-2009. An increase in the drilling rate[5] resulted in a minor overall increase in the intermediate CRA-2009 PA cuttings and cavings releases, as compared with the PABC-2004 results (DOE 2009, Appendix PA, Section PA-9.1). However, this minor increase was subsequently offset by a small decrease in the PABC-2009 releases at probabilities below 0.001 due to an updated waste radionuclide inventory that was lower after roughly 350 years and remained lower for the rest of the 10,000-year regulatory period (Clayton et al. 2010, Section 6.1).

11.2   DIRECT BRINE RELEASE CALCULATIONS

A direct brine release (DBR) occurs when contaminated brine originating in the repository is driven up an intrusion borehole to the ground surface by repository gas pressure. A DBR occurs only when the repository gas pressure exceeds the estimated 8 MPa hydrostatic pressure of the drilling fluid and the brine saturation exceeds the residual saturation of the waste material (Leigh et al. 2005a, Section 3.7). The BRAGFLO code is used in WIPP PA with a two-dimensional plan view grid that dips 1° to the south to calculate DBRs. Inputs to the BRAGFLO code for DBR calculations include the location of the drilling penetration in the repository (either an up-dip, a middle, or a down-dip location is selected). Inputs also include repository conditions at the time of penetration such as gas/brine pressure and brine saturation. A set of 100 vectors is run for each replicate/drilling scenario/intrusion time/intrusion location combination (Long 2008, Section 5.7). Volume-weighted averages of repository conditions (pressure, saturation, porosity, and crushed waste panel height) at the time of penetration are taken from the CUTTINGS_S code (Vugrin and Fox 2005, Section 2) and used to interpolate DBR volumes calculated by BRAGFLO for a given realization. This approach was found to provide sufficient accuracy and was used in the 2009 PAs, as well as in the 2004 and earlier PAs. The radiological properties of the DBR volumes are calculated by the CCDFGF code (Long 2008, Sections 5.9.3 and 5.10).

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[5] The reader is referred to EPA 2010f for the Agency's review of changes in the drilling rates since the PABC-2004.

11.2.1 Modifications since the PABC-2004

BRAGFLO Version 4.10 was used for calculating DBR volumes for the PAVT; BRAGFLO Version 5.0 was used for calculating DBR volumes for the PABC-2004; and BRAGFLO Version 6.0 was used for calculating DBR volumes for both the intermediate CRA-2009 PA (Long 2008, Table 4.1) and the PABC-2009 (Long 2010, Table 4.1). The modifications made in the Version 5.0 revision are summarized in EPA 2006c, Section 10.2.1. Version 6.0 is identical to Version 5.0, except that subroutines have been added to model capillary pressure at brine saturations below residual saturation, as well as chemical reactions involving iron and magnesium. In addition, enhancements were made in the treatment of material changes in the repository, host rock and intrusion boreholes. The functional requirements for BRAGFLO Version 6.0 include all those specified for BRAGFLO Version 5.0 plus the following additional functionality (Nemer 2007a and 2007b).

- The initial concentration of MgO was added as a functional requirement to model MgO hydration.

- Chemical reactions within the repository influence repository pressure and brine saturation.

- Chemical reactions can be stopped when materials change as specified by the .INP input file.

- Five additional chemical reactions are modeled: sulfidation of iron hydroxide; sulfidation of iron, hydration of MgO, carbonation of $Mg(OH)_2$; and carbonation of MgO. Stoichiometry is specified for each of these reactions in the input file (.INP).

- Reaction rates for all chemical reactions are set to zero when brine saturation drops below a specified minimum value, which is set in the input file.

- Reaction rates for all chemical reactions are multiplied by their respective initial concentrations if specified by a flag in the .INP input file.

- Changes in solid volume resulting from the chemical reactions are calculated.

- Capillary pressure is modeled at brine saturations below residual saturation.

- A new subroutine RESETMID has been added to reset the saturation, pressure, and concentrations in a material at the time of a material change.

- Material changes are accompanied by smooth changes in permeability with time, as specified by the input file.

Although the functionality to simulate additional chemical reactions involving iron and magnesium was added to BRAGFLO Version 6.0, this functionality was not used in the CRA-2009 or the PABC-2009. Only microbial degradation of organic materials and corrosion of steel were modeled (DOE 2009, Appendix PA-2009 Performance Assessment, p. PA-64; EPA 2010e, Section 3.0). The Agency considers the foregoing modifications to the BRAGFLO code to be appropriate. Validation of BRAGFLO Version 6.0 was reviewed in EPA 2010c.

11.2.2 DBR Calculation Results

Only a fraction of realizations result in direct brine flow to the ground surface because of the dependence of brine releases on repository pressure and brine saturation. The conditions needed for a DBR to occur have been found to be only slightly different among the three replicates (Stein et al. 2005, Section 6). Using Replicate R1 as an example, 996 of the 7,800 DBR calculations (or about 13%) in the PABC-2009 PA resulted in direct brine flow to the surface (Clayton 2010, Section 6.1). Although the maximum brine release volume in Replicate R1 was 42 m^3, the average nonzero release was only 0.9 m^3 (Clayton et al. 2010, Table 5-5). In general, release volumes were low or zero when the pressure and brine saturation were both low, but release volumes were also low when brine saturation was high because of the reduced relative permeability to gas flow (Clayton et al. 2010, Section 5.5.4).

Comparable DBR results for the PABC-2004 are presented in Leigh et al. 2005a, Section 5.5.3. For PABC-2004 Replicate R1, 721 of the 7,800 DBR calculations (or about 9%) resulted in direct brine flow to the surface. The maximum DBR release in Replicate R1 was approximately 69 m^3. While maximum release volumes are sensitive to the specific combination of repository pressure and brine saturation at the time and location of the drilling intrusion and are therefore variable, the average nonzero releases remained much lower (see, for example, Leigh et al. 2005a, Figures 5-48 through 5-52).

Figure 11-2 illustrates the differences between the normalized DBR radionuclide releases for the PABC-2004 and PABC-2009, expressed as the combined mean complimentary cumulative distribution functions (CCDFs) for all three replicates. Comparison of these curves shows that the mean brine radionuclide releases in the PABC-2009 were higher than in the PABC-2004 at all probabilities. This increase is primarily attributed to an increase in the number of brine releases and in the release volumes due to increases in repository pressure (affecting the intermediate CRA-2009 PA; DOE 2009, Appendix PA, Section PA-9.3), combined with a subsequent increase in the concentration of actinides in the brine resulting from higher radionuclide solubility limits (affecting the PABC-2009 PA; Clayton et al. 2010, Section 6.3). DOE attributes the higher pressure to increased brine availability associated with higher intact halite porosities (DOE 2009, Appendix PA, Section PA-9.3). Higher radionuclide solubilities are the result of increased organic ligands in the PABC-2009 inventory. A contributing but less significant increase in DBR volumes resulted from the aforementioned increase in the drilling rate. Given these changes, the calculated increase in DBR radionuclide releases is reasonable.

11.3   SPALLINGS CALCULATIONS

Spallings releases occur when solid waste is ejected through an intrusion borehole by repository gas pressures that exceed the estimated 8 MPa hydrostatic pressure of the drilling fluid (Vugrin 2005b, Section 2.0). The rapid release of highly pressurized repository gas during repository penetration by a borehole can cause localized mechanical failure and entrainment of solid waste as the gas moves into and through the borehole. The DRSPALL code is used in WIPP PA to calculate spallings release volumes. Inputs to the DRSPALL code include borehole characteristics such as length, diameter and drilling rate; the repository gas pressure; and physical properties of the waste including permeability, porosity, tensile strength and particle

diameter after tensile failure. The DRSPALL code is used to calculate spallings release volumes for four initial reference values of repository gas pressure (10, 12, 14, and 14.8 MPa) for a single drilling intrusion (Ismail 2010, Section 2.3). The actual release volume used in a PA calculation for a given borehole intrusion is interpolated from these reference results by the CUTTINGS_S code using the repository gas pressure calculated by BRAGFLO at the time of intrusion. This volume is multiplied by the average repository radionuclide activity and the fraction of the repository occupied by waste to estimate the spallings radionuclide release. The radiological properties of the spallings release volumes are calculated by the CCDFGF code (Vugrin 2005a, Section 2.2).

11.3.1 Modifications since the PABC-2004

DRSPALL was developed for the CRA-2004 PA to replace the original SPALLINGS code used as a basis for the range of spallings volumes sampled in the PAVT. DRSPALL Version 1.0 was used in the CRA-2004 PA and Version 1.1 was used in the PABC-2004 (Vugrin 2005b, Section 2.0). The conceptual basis for the DRSPALL code was reviewed and approved by an independent peer panel (Yew et al. 2003; Yew 2004). Two additional sensitivity studies made at the Agency's request (EPA 2004a, Comments G-8-1 and G-8-2; see DOE responses in DOE 2004a and DOE 2004c) also had positive outcomes.

DRSPALL includes the option to specify either a hemispherical or a cylindrical spallings cavity. A spherical geometry is nominally selected for WIPP PA because it better represents the shape of small cavities. However, in realizations that result in larger cavities, the cavity radius can exceed the height of the repository. In such situations, DRSPALL is restarted in the cylindrical mode with an initial radius specified to be the height of the repository to account for the cavity created when DRSPALL was run in the spherical mode (Vugrin 2005b, Section 4.2.4). The differences between DRSPALL Version 1.0 and Version 1.1 are procedural rather than technical and include a modified sampling procedure for uncertain parameters, an increased number of vectors per replicate, and use of a new input file utility code. Additional discussion of these changes is presented in EPA 2006a, Section 10.3.1. Given approval of the DRSPALL conceptual model by an independent peer review panel, the positive outcomes of two additional sensitivity studies requested by the Agency, and the successful DOE validations, the Agency concludes that the DRSPALL code is appropriate for use in WIPP PA.

DOE did not rerun the DRSPALL code for either the intermediate CRA-2009 PA (Long 2008, Section 5.5) or the PABC-2009 (Long 2010, Section 5.6), and instead used the same results as calculated for the PABC-2004. This was appropriate because none of the updates or corrections for the 2009 PAs affected the DRSPALL calculations.

11.3.2 Calculation Results

As stated above, the DRSPALL results for the PABC-2004 were also used for the PABC-2009. The spallings release volumes calculated by DRSPALL for the four previously mentioned initial repository reference pressures used for the PABC-2004 are presented in Section 5.5.2 of Leigh et al. 2005a. These pressures correspond to what are referred to as DRSPALL pressure scenarios (Vugrin 2005b, Section 4.2). As expected, mean spall volumes increased with increasing initial repository gas pressures and amounted to 0.172 m^3 at 12 MPa, 0.665 m^3 at 14 MPa, and

0.978 m^3 at 14.8 MPa (Leigh et al. 2005a, Table 5-6). Maximum spall volumes ranged from 7.71 m^3 at 12 MPa to 14.5 m^3 at 14.8 MPa (Leigh et al. 2005a, Table 5-6). No spallings releases occurred at an initial repository gas pressure of 10 MPa. Because the spallings release volume for a given borehole intrusion is interpolated from these reference results using the repository gas pressure calculated by BRAGFLO at the time of intrusion, the predicted spallings release volumes for the PABC-2009 will not necessarily be the same as for the PABC-2004.

Actual maximum spallings volumes used in the PABC-2004 are presented in Leigh et al. 2005a, Section 5.5.2.2. The maximum total spallings release volumes in the three replicates of the PABC-2004 ranged from 0.80 m^3 to 8.33 m^3 (Leigh et al. 2005a, Table 5-7). Of the 7,800 spallings volumes calculated per replicate for the PABC-2004, more than 94% of each replicate's calculations resulted in no spallings (Leigh et al. 2005a, Section 5.5.2.2).

Actual spallings volumes used in the PABC-2009 were calculated using the PABC-2004 reference volumes calculated by DRSPALL and interpolated to the PABC-2009 repository pressures calculated by BRAGFLO at the time of drilling intrusion. Of the 7,800 spallings volumes calculated per replicate in the PABC-2009, more than 93% of each replicate's calculations resulted in no spallings (Clayton et al. 2010, Section 5.5.3). While the maximum total spallings release volumes in the three replicates of the PABC-2009 ranged from 2.76 m^3 to 8.29 m^3, the average nonzero spallings release volume ranged from only 0.38 m^3 to 0.43 m^3 (Ismail 2010, Table 7).

The waste permeability, waste porosity, waste tensile strength and waste particle diameter after tensile failure are treated as uncertain parameters in the DRSPALL model. The largest spall volumes occurred when the waste permeability was low. This is because the lower permeability leads to increased resistance to gas flow through the waste, resulting in greater tensile stresses and waste tensile failures. Smaller particle diameters also led to larger spall volumes because the smaller particles could be transported more easily by the escaping repository gas. These results are reasonable and consistent with the spallings conceptual model.

Although spallings releases in a given borehole intrusion could exceed 10 m^3 and could therefore be larger than the largest cuttings and cavings release of 3.41 m^3 in the PABC-2009, the frequency of spallings release in both the PABC-2004 and PABC-2009 was low because of its dependency on repository gas pressure. Spallings were therefore not large contributors to total releases in either PA.

Figure 11-3 illustrates the differences between the normalized spallings radionuclide releases for the PABC-2004 and PABC-2009, expressed as the combined mean complimentary cumulative distribution functions (CCDFs) for all three replicates. Comparison of these curves shows that the mean spallings releases in the PABC-2009 were slightly higher than in the PABC-2004 PA at probabilities above 0.01. Spallings volumes increased between the PABC-2004 and the intermediate CRA-2009 PA primarily due to the aforementioned increase in repository pressure, with a smaller contribution due to the increased drilling rate (DOE 2009, Appendix PA, Section PA-9.2). The spallings volume increases seen in the CRA-2009 PA were subsequently reduced in the PABC-2009 by a small reduction in repository pressure attributed to a reduced inventory of CPR materials which, when degraded by microbial activity, release gas into the repository (Ismail 2010, Section 4.2.1). In addition to the spallings volume decreases, the spallings

radionuclide releases decreased in the PABC-2009 as a result of the aforementioned updated waste radionuclide inventory that was lower after roughly 350 years and remained lower for the rest of the 10,000-year regulatory period than in the CRA-2009 PA (Clayton et al. 2010, Section 6.2).

11.4 PABC-2004 AND PABC-2009 DIRECT RELEASE COMPARISONS

Comparison of Figures 11-1 through 11-3 shows that normalized direct radionuclide releases are dominated by cuttings and cavings releases at probabilities above approximately 0.01 and by DBRs at probabilities below approximately 0.01. This is because cuttings releases occur in every intrusion but in relatively low volumes, while DBRs occur less often but can occasionally occur in sufficiently large volumes to support larger radionuclide releases. Spallings releases can occur in larger volumes than cuttings and cavings releases, but the frequency of spallings releases is low and, consequently, spallings are not large contributors to total releases.

Figures 11-1 through 11-3 show that the mean normalized radionuclide releases for each of the three direct release mechanisms evaluated in the PABC-2009 are at least an order of magnitude less than the normalized Agency release limits at probabilities of 0.1 and 0.001. Given that the direct release models have been found to be reasonable and appropriate for WIPP PA, the Agency concludes that the direct release modeling results are also reasonable and appropriate. Total releases modeled for the PABC-2009 are discussed and compared to both calculated PABC-2004 releases and regulatory release limits in Section 12.0.
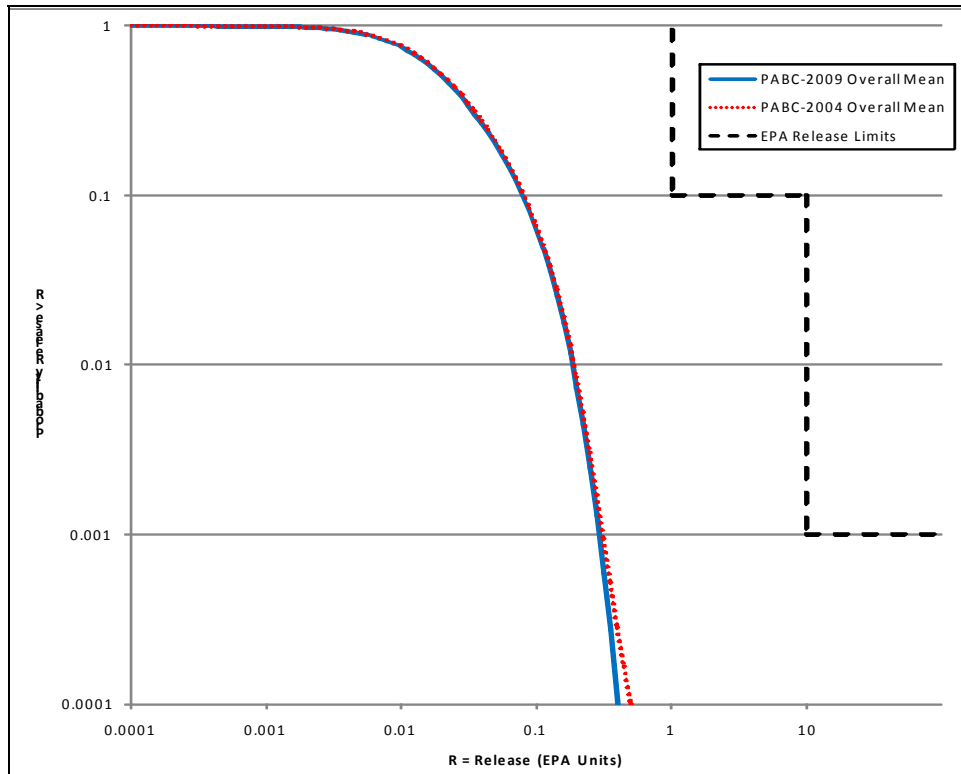
Figure 11-1. Overall Mean PABC-2004 and PABC-2009 CCDFs for Cuttings and Cavings Releases

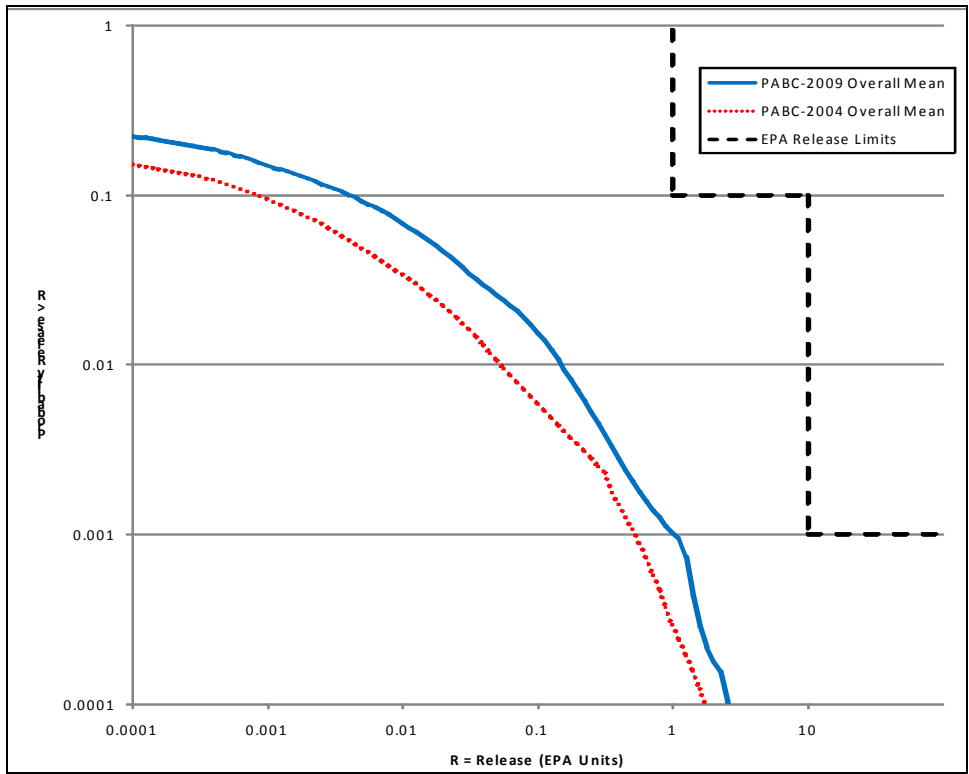(Source: Camphouse 2010a, Figure 1)

Figure 11-2. Overall Mean PABC-2004 and PABC-2009 CCDFs for Direct Brine Releases

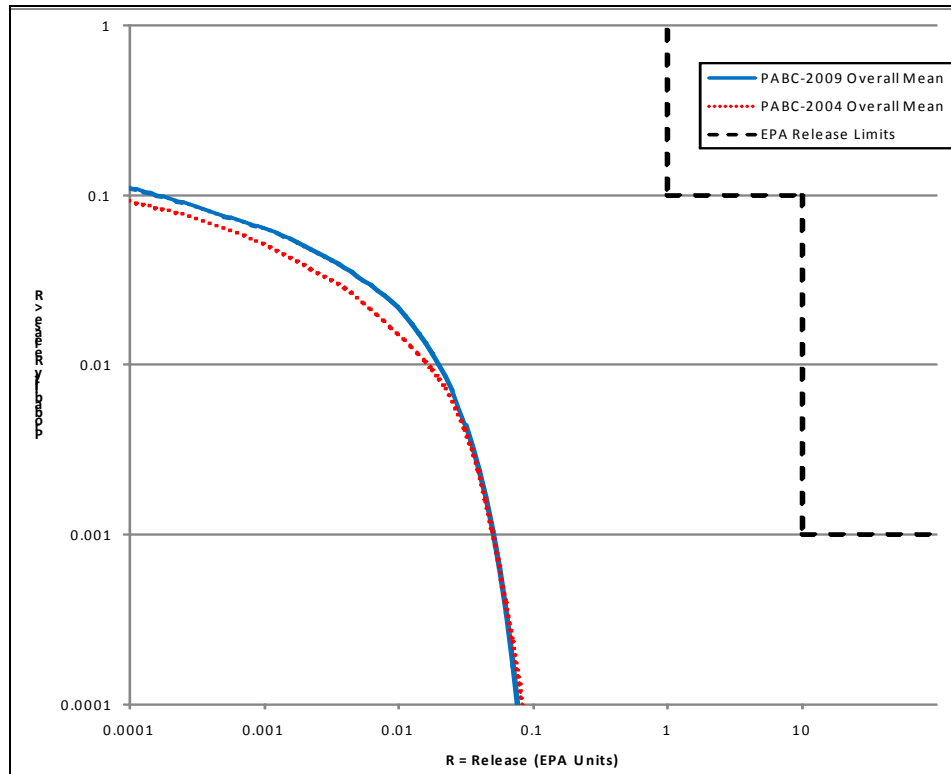(Source: Camphouse 2010a, Figure 3)

Figure 11-3.   Overall Mean PABC-2004 and PABC-2009 CCDFs for Spallings Releases

(Source: Camphouse 2010a, Figure 2)

12.0   RESULTS OF PABC-2009 CALCULATIONS

PABC-2009 calculations were performed by the DOE to address the Agency's Containment Requirements (40 CFR 191.13), Individual Protection Requirements (40 CFR 191.15), and Groundwater Protection Requirements (40 CFR Part 191, Subpart C). In this section, the PA results are reviewed in the context of contributing release pathways and total releases. Undisturbed pathways (Section 12.1) are those that occur when there are no unlikely natural events or human intrusions into the repository and are used when addressing the Individual and Groundwater Protection Requirements. Human intrusion occurs when, for example, exploratory oil and gas boreholes disrupt the repository by intersecting the repository waste and creating new release pathways. These are called disturbed pathways (Section 12.2). Releases through both undisturbed and disturbed pathways are addressed in the Agency's Containment Requirements. The releases of the various radionuclides are normalized according to a procedure specified by the Agency (40 CFR Part 191, Appendix A). The normalized releases for undisturbed and disturbed pathways are then summed to project total releases for comparison with the Agency's Containment Requirements (Section 12.3). Upon completing the PA calculations, DOE performed a sensitivity analysis to determine which parameters used in PA have the greatest influence on the results (Section 12.4).

12.1   UNDISTURBED PATHWAYS

DOE has identified two credible pathways for the S1 (undisturbed pathways) scenario by which radionuclides could reach the accessible environment under undisturbed conditions (Leigh et al. 2005a, Section 4.1.3):

(1) Radionuclide transport may occur laterally, through anhydrite interbeds toward the subsurface boundary of the accessible environment in the Salado Formation.

(2) Radionuclide transport may occur through access drifts or anhydrite interbeds to the base of the WIPP shafts. In this case, if the pressure gradient between the waste panels and overlying strata is sufficient, contaminated brine may migrate up the shafts and then be transported laterally away from the shafts, through permeable strata such as the Culebra, toward the subsurface boundary of the accessible environment.

The Agency concurs with this selection of pathways and notes that these pathways were also included in the prior PAs, including the Agency-mandated PAVT, PABC-2004, and CRA-2009. These pathways are discussed in more detail in Sections 8 and 10. For both pathways, brine flow is driven by high repository pressures.

12.1.1 Lateral Transport through Anhydrite Interbeds

Small volumes of brine were calculated in the PABC-2004 analysis to cross the Land Withdrawal Boundary (LWB) and enter the accessible environment by flowing through the anhydrite interbeds under undisturbed conditions. The maximum of any vector in Replicate 1, for example, was about 1,200 m^3 (Leigh et al. 2005a, Figure 4-17). Only one vector in the undisturbed PABC-2004 analysis was found to have the potential for the transport of

radionuclides through the interbeds from the repository to the LWB. The maximum total integrated discharge across the land withdrawal boundary by this pathway in the undisturbed PABC-2004 analysis was 1.31×10^{-12} EPA units (Leigh et al. 2005a, Section 4.2.2). DOE noted that a release of this magnitude is smaller than the effective numerical precision of the transport calculations when numerical dispersion is considered (Leigh et al. 2005a, Section 4.2.2).

In the PABC-2009, the maximum brine volume crossing the WIPP LWB was about 1,360 m^3. (Clayton et al. 2010, Section 4.1.3). Only one vector showed radionuclide transport across the LWB – Replicate 1, Scenario S1, Vector 53 – 6.3 x10^{-11} EPA units. This quantity of radioactivity is inconsequential. The small undisturbed releases calculated through anhydrite interbeds in the PABC-2009 are consistent with the small releases calculated in the PABC-2004.

12.1.2 Transport through Shafts

Brine moving up the shaft and entering the Culebra is not necessarily contaminated with radionuclides because it may not have been in contact with the waste. In the PABC-2009 analysis, no radionuclides were calculated to be transported up the shafts and through the Culebra to the accessible environment under undisturbed conditions (Clayton et al. 2010, Section 4.2.1). Brine flow up the shaft in the PABC-2004 analysis was also insignificant (Leigh et al. 2005a, Section 4.2.1).

12.1.3 Comparison with Individual Protection Standard

The Individual Protection Standard contained in 40 CFR 191.15 limits the maximum annual committed effective dose to an individual outside the LWB to 15 millirem. Undisturbed releases applicable to this standard can occur through the overlying Culebra dolomite via brine flow from the repository through the WIPP shafts or from lateral, subsurface brine migration to the accessible environment through anhydrite interbeds within the Salado repository host formation. In both the undisturbed PABC-2004 and PABC-2009 analyses, brine flow up the shaft was insignificant and releases through the anhydrite interbeds were small and likely due to model limitations resulting from numerical dispersion. The Agency therefore considers that the Individual Protection Standard continues to be met.

12.1.4 Comparison with Groundwater Protection Standard

The Groundwater Protection Standard contained in 40 CFR 191.24(a)(1) states the following:

> *General. Disposal systems for waste and any associated radioactive material shall be designed to provide a reasonable expectation that 10,000 years of undisturbed performance after disposal shall not cause the levels of radioactivity in any underground source of drinking water, in the accessible environment, to exceed the limits specified in 40 CFR Part 141 as they exist on January 19, 1994.*

The National Primary Drinking Water Standards are specified by the Agency in 40 CFR 141. Both undisturbed release pathways considered in WIPP PA have the potential to affect the groundwater. The drinking water requirements of 40 CFR 141.66 require that the combined concentrations of Ra-226 and Ra-228 be less than 5 pCi/L in any underground source of drinking

water through 10,000 years. For PABC-2009 the radium concentration was 0.0006 pCi/L—a value well below the regulatory limit (Clayton et al. 2010, Section 4.2.2). The Agency therefore considers that the Groundwater Protection Standard continues to be met.

12.2   DISTURBED PATHWAYS

The DOE has identified four credible pathways by which radionuclides could reach the accessible environment (Leigh et al. 2005a, Section 5) in disturbed scenarios as described below. The Agency concurs with this selection of pathways and notes that they were also included in the prior PAs. The four additional pathways consist of radionuclide releases via exploratory oil and gas boreholes that intersect repository waste. The first three of these additional pathways involve direct releases and account for most calculated repository releases. These were discussed in more detail in Section 11. The fourth pathway considers releases of contaminated brine through a plugged borehole into the Culebra. These four pathways are characterized as follows:

(1) Radionuclides may be transported to the ground surface as borehole cuttings and cavings. These are the solid materials removed from the repository and carried to the ground surface by drilling fluid during the process of drilling a borehole that intersects repository waste. Cuttings are the waste materials removed directly by the drill bit, and cavings are the waste materials eroded from the borehole wall by shear stresses from the circulating drilling fluid.

(2) Radionuclides may be transported to the ground surface when contaminated brine originating in the repository is driven up an intrusion borehole to the ground surface by repository gas pressures that exceed the estimated 8 MPa hydrostatic pressure of the drilling fluid. These are called direct brine releases (DBRs).

(3) Radionuclides may be transported to the ground surface when solid waste is ejected through an intrusion borehole by repository gas pressures that exceed the estimated 8 MPa hydrostatic pressure of the drilling fluid. These are called spallings releases.

(4) Radionuclides may be transported up to the Culebra dolomite through a degraded borehole seal and subsequently transported by moving groundwater through the Culebra to the subsurface boundary of the accessible environment.

These pathways, which involve two drilling scenarios individually or in combination, have been included in all PAs. In the first scenario (E1) the borehole is assumed to pass through the repository and encounter a pressurized brine reservoir in the underlying Castile Formation. In this scenario, the borehole acts as a conduit connecting the brine reservoir with the repository and the repository with the ground surface. In the second scenario (E2), the borehole is assumed to pass through the repository but does not encounter an underlying pressurized brine reservoir. In addition, the potential effects of mining for potash within the land withdrawal boundary on altering groundwater flow patterns in the Culebra are also considered.

12.2.1 Direct Releases

Direct radionuclide releases to the ground surface occur through cuttings and cavings, direct brine and spallings releases. The calculated combined mean contributions of these release pathways to total releases are shown for the three replicates of the PABC-2009 in Figure 12-1. These three release pathways account for essentially all of the calculated repository releases at higher probabilities (i.e., >0.01). Cuttings and cavings releases have changed little since the PAVT and continue to comprise the dominant release pathway at high probabilities. This is because contaminated drill cuttings are projected to be released to the ground surface in every intrusion borehole, and cavings releases are projected to occur in most intrusion boreholes. Calculated direct brine releases have increased significantly since the PAVT, particularly at low probabilities where they have become the dominant release pathway. This is primarily due to higher brine saturations resulting from lower microbial gas generation rates, and to changes in the PABC-2009 that increased actinide solubilities. Calculated spallings releases have decreased significantly since the PAVT at both high and low probabilities. This reduction was in part due to the new DRSPALL model, but was also in part due to reduced long-term microbial gas generation rates and consequent lower repository pressures.

12.2.2 Releases through the Culebra

Calculation of releases through the Culebra takes into account not only the effects of the intruding borehole(s) but also effects of potash mining in the McNutt Potash zone of the Salado Formation underlying the Culebra and overlying the WIPP repository. Subsidence associated with potash mining can cause additional fracturing in the Culebra dolomite increasing transmissivity and consequent releases to the land withdrawal boundary. Two modeling approaches are used to include mining effects. The partial mining scenario assumes that mining only occurs outside the LWB while the full mining scenario considers mining both inside and outside the LWB.

In the PABC-2009, releases for the partial mining scenario were minimal as shown in Table 12-1 with only U-234 (37 of 300 vectors) and its daughter Th-230 (21 of 300 vectors) showing a significant number of vectors with cumulative releases over the 10,000-year regulatory period above a threshold of 10^{-9} kg over the (Kuhlman 2010, Table 4-5). In this table, Th-230 is the ingrowing daughter of U-234 while Th-230A is the initially present radionuclide in the waste.

Table 12-1.   Number of Vectors In for Each PABC-2009 Replicate with Releases through the Culebra to the LWB

Radionuclide	Partial Mining			Full Mining		
	R1	R2	R3	R1	R2	R3
Am-241	0	0	0	8	10	3
Pu-239	3	1	1	20	27	22
U-234	11	14	12	48	50	47
Th-230	5	10	6	36	38	42
Th-230A	2	3	0	21	31	29

Substantially greater releases for all radionuclides in all replicates occur in the full mining case (e.g., 145 of 300 vectors for U-234). Uranium-234 and its daughter Th-230 had the largest cumulative masses transported to the Culebra to the LWB. Releases to the Culebra are significantly greater in the PABC-2009 than in the PABC-2004. DOE attributes this to three factors (Kuhlman 2010, Section 4.3):

- Speedup due to mining. The definition of mineable potash provided by the BLM has changed considerably, especially within the LWB. This is discussed in more detail in EPA 2010f. Mineable potash ore is now located within about 670 m of the center of the waste panels.

- Speedup due to decreases in retardation coefficients. The lower limits of retardation coefficients were reduced several orders of magnitude for most radionuclides except U(VI) as required by EPA. The requirement was driven by increased organic ligands in the waste inventory.

- Speedup due to MODFLOW calibration. A high-transmissivity zone is present in the Southeastern portion of the WIPP site in all calibrated MODFLOW realizations. Presence of the zone was confirmed by pump tests in well SNL-14.

EPA concurs with this assessment.

Mean normalized releases based on disturbed case transport through the Culebra are shown in Figure 12-2 and are compared with Replicate 2 of the CRA-2009 (Camphouse 2010b, Figure 3-27). While not shown in Figure 12-2, Replicate 2 for the CRA-2009 PA is virtually identical to Replicate 2 of the PABC-2004 (Dunegan 2008, Figure 4.40), clearly demonstrating increased releases via this pathway in the PABC-2009.

12.2.3 Releases through Anhydrite Interbeds

Releases of radionuclides through the anhydrite interbeds were inconsequential in the disturbed case scenarios. No vectors in the 300 realizations in the PABC-2009 resulted in transport of radionuclides exceeding 10^{-10} EPA units through the anhydrite interbeds and across the land withdrawal boundary under disturbed conditions (Ismail and Garner 2010, Section 4.1.2). The largest release was 6.3E-11 EPA units for an E1 intrusion at 100 years. In many cases these very small releases are numerical artifacts.

12.3   TOTAL NORMALIZED RELEASES

Total normalized releases are calculated by summing the releases from each pathway including cuttings and cavings releases, DBRs, spallings releases and releases from the Culebra. There were no releases from transport up the shaft and only miniscule releases through the anhydite layers for the undisturbed case in the PABC-2009. Consequently, the undisturbed pathways (S1 scenario) were excluded from the calculation of total normalized releases.

Combined mean normalized releases from the four primary release pathways for the PABC-2004 and PABC-2009 calculations are compared in Table 12-2 at the Agency's regulatory probability

measurement points of 0.1 and 0.001. In addition, total combined mean normalized releases for the PABC-2004, CRA-2009 and PABC-2009 calculations are compared in Figures 12-3 and 12-4. The combined mean CCDF is computed as the arithmetic mean of the three mean CCDFs from each replicate. It is noted that the total releases are less than the sum of the component releases at the given probabilities. This is because the ranked percentiles generally correspond to different realizations for the individual release mechanisms, whereas the total releases represent the combination of all release mechanisms that occur in a given realization.

For the CRA-2009 PA, Figure 12-3 shows a small increase as compared to PABC-2004. DOE attributes this to an increase in the drilling rate (DOE 2009, Section 2.1.6; EPA 2010f). For PABC-2009, Figure 12-4 shows a small decrease as compared to the CRA-2009 PA at high probabilities, which is attributed to a decrease in cuttings and cavings and a small increase at low probabilities related to greater direct brine release and Culebra transport in the PABC-2009. The cuttings and cavings decrease is, in turn, attributed to the revised inventory used in the PABC-2009. The increase in DBR in PABC-2009 stems from increases in the solubility limits primarily for +III valence elements, which are driven by higher concentrations of organic ligands in current waste inventory (See Table 3-6). Releases driven by transport through the Culebra are also significantly higher in the PABC-2009 than in prior PAs. This effect is more prominent at low probabilities. Factors contributing to increased Culebra releases include higher actinide mobilization as a result of increased organic ligand concentrations, reduced K_d values along the flow path and increased transmissitivity resulting from possible subsidence from potash mining closer to the waste panels.

As can be seen from Table 12-2, for the PABC-2009, both the calculated mean releases and the upper 95% confidence levels on the mean have remained less than the regulatory limits at both 0.1 and 0.001 probabilities. Therefore, the Agency concludes that the WIPP continues to comply with the containment requirements of 40 CFR 191.13.

Table 12-2.   Combined Mean Releases for All Replicates

Release Mechanism	Mean Release in EPA Units at Probability = 0.1		Mean Release in EPA Units at Probability = 0.001	
	PABC-2004	**PABC-2009**	**PABC-2004**	**PABC-2009**
Mean Total Releases	0.09	0.09	0.60	1.10
Upper 95% Confidence Level	0.09	0.10	0.68	1.77
Regulatory Limits	1.00	1.00	10.0	10.0

Sources: DOE 2009, Table PA-35 and Clayton et al. 2010, Table 6-1.
EPA confidence level requirement from 40 CFR § 194.34(f).
EPA regulatory limits from 40 CFR 191.13(a).

12.4   SENSITIVITY ANALYSIS

Stepwise rank regression analyses were used by DOE to evaluate the sensitivity of the normalized releases to the sampled parameters. The results of these analyses for the PABC-2004 are presented in Leigh et al. 2005a (Section 7), and the results for the PABC-2009 and the CRA-2009 PA are presented in Kirchner 2010a. These analyses compare the sampled input parameter values with the calculated release data to rank the relative importance of the parameters to the

calculated releases. The calculated release is considered sensitive to a parameter if changes in the parameter value over its range of uncertainty result in large changes in the calculated release. The analysis results are limited to parameters that were treated as epistemic uncertainties in the PA.

Because cuttings, cavings, direct brine and spallings releases account for an overwhelming majority of the total releases, the calculated total releases are most sensitive to uncertainties in the parameters governing these release mechanisms. The calculated total releases were found to be most sensitive to the parameters listed in Table 12-3. Increasing sensitivity is indicated by increasing absolute values of the standardized rank regression coefficients (SRRCs) and high correlation coefficient (R^2) values. In all of the PAs, total normalized releases were most sensitive to uncertainty in waste shear strength (WTAUFAIL), which is a key parameter governing cavings volumes. The negative correlation found for WTAUFAIL in the analysis indicates increasing releases with decreasing shear strengths, and is expected.

In the PAs, direct brine releases supplant spallings as the second most important contributor to total releases and even surpass cuttings and cavings at low probabilities (Figure 12-1). The second most important variable in the PAs is WSOLVAR3, a solubility multiplier that characterizes uncertainty in solubilities for all actinides in the +3 oxidation state. This parameter increases the radionuclide concentration in direct brine releases. The drill string angular velocity (DOMEGA), used in computing cavings releases, appears third in PABC-2004, but is less significant in Replicate 1 in the CRA-2009 PA and in the PABC-2009.

Each of the remaining parameters in Table 12-3 for the PABC-2009 sensitivity analysis explains less than 2% of the variability in the total releases and is therefore not particularly significant to total uncertainty. WFBETCEL is a scale factor used in defining the stoichiometric coefficient for microbial gas generation; BPINTPRS is the initial brine pore pressure in the Castile brine reservoir; PBRINE is the probability that a drilling intrusion penetrates a Castile brine reservoir; SHURGAS is the residual gas saturation in the upper shaft seal materials; and SHLPRM2 is the permeability of the lower shaft seal materials for the first 200 years after repository closure. Most of these parameters affect brine saturation and repository gas pressure, which have important roles in direct brine and spallings releases. The presence of the parameters SHURGAS and SHLPRM2 on this list is probably the result of statistical noise because no releases were calculated to occur through the shafts. CTRAN is an index used to select one of 100 equally probable transmissivity fields for the Culebra dolomite.

In reviewing the PABC-2009 sensitivity analysis, the Agency noted that the parameter WFBETCEL (also described as CELLUS:FBETA) was the third listed parameter in stepwise regression analysis for Replicate 1 of both the PABC-2009 and CRA-2009 (Kirchner 2010b Table 4), but this parameter did not appear among the top seven parameters for Replicates 2 and 3 of PABC-2009. According to Kirchner, this indicates "that its correlation may not be a reliable indicator of importance." This anomalous behavior suggested that the role of the parameter be investigated further.

As part of this investigation, EPA submitted Technical Comment 1 to DOE (Byrum 2010). This comment is summarized below.

According to the parameter data sheet in CRA-2004 (DOE 2004b, Appendix PA, Attachment PAR, Parameter 5), "Factor beta is an index that characterizes the stoichiometry used to calculate the microbially generated gas, accounting for the interaction with gases reacting with steel and steel corrosion products." The variable β as defined in the following equation was treated as an uncertain quantity in the CRA-2004 PA (DOE 2004b, Appendix PA, Section PA-4.2.5):

$$y = y_{min} + \beta(y_{max} - y_{min}), 0 \leq \beta \leq 1.$$

The parameter y is the average stoichiometric factor in the generalized equation for microbial degradation of CPR materials:

$$C_6H_{10}O_5 + \text{unknowns} = 6y \text{ (mol) gas} + \text{unknowns}.$$
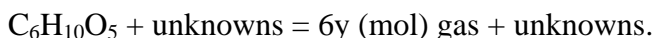
The parameter y represents the number of moles of gas produced and retained in the repository for each mole of carbon consumed in biodegradation reactions, and depends on the extent to which biodegradation reactions occur along particular pathways (i.e., denitrification, sulfate reduction and methanogenesis) and the extent to which the CO_2 reaction product is consumed by MgO.

For the PABC-2004 and subsequent PAs, EPA required that methanogenesis not be considered as a biodegradation reaction based on the premise that sufficient sulfate was present in the repository to continue to promote the sulfate reduction reaction. In response to this requirement, DOE revised the equations to calculate the average stoichiometric factor y (Nemer and Zelinski 2005). Nemer and Zelinski (2005, Section 4.3) state that: "Thus y and β are no longer sampled input parameters."

Although the gas generation model was the same for the CRA-2009 PA and PABC-2009 as was used in PABC-2004, WFBETCEL continues to appear as a parameter contributing to uncertainty. This is in spite of the statement that β is no longer a sampled input parameter.

In its response, to Technical Comment 1, DOE noted that (Patterson 2010):

- The parameter CELLULS:FBETA will be removed from the parameter sampling in future calculations.

- The text in Nemer and Zelinski (2005) will be rewritten as, "*Thus β is no longer needed as a sampled input parameter. However, the parameter y will still be sampled indirectly as it depends on the sampled parameter WAS_AREA:PROBDEG through the variable M'$_{cel}$.*"

- The parameter CELLULS:FBETA is not contained in the top seven correlation parameters for Replicates 2 and 3, and no correlations with that parameter were found for any of the individual release pathways for Replicates 1, 2 or 3, which further illustrates that the correlation is spurious.

- These items will be noted as errata to the "*Sensitivity of the 2009 CRA Performance Assessment Baseline Calculation Releases to Parameters.*" document.

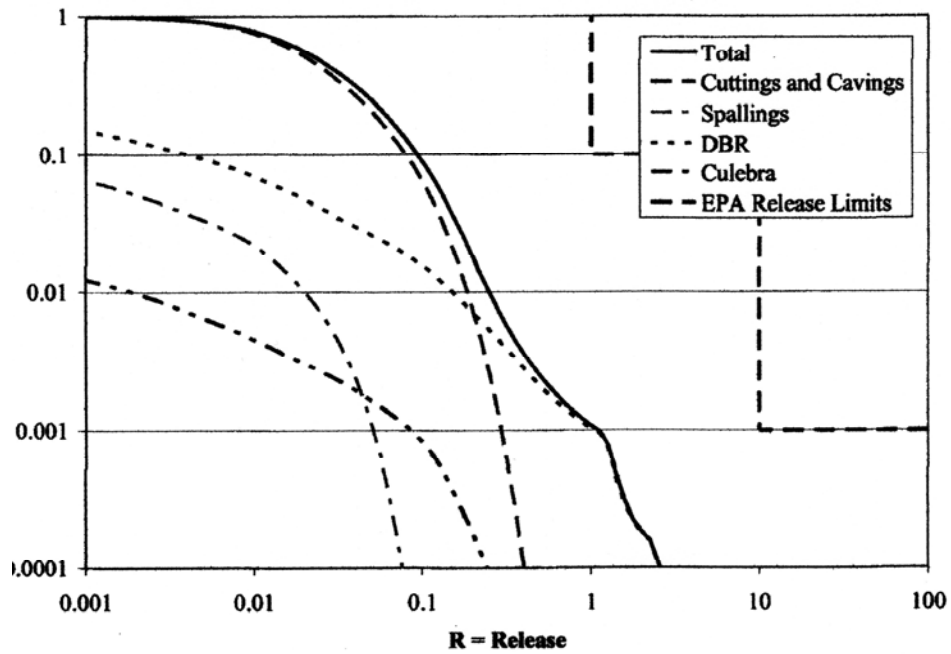EPA is satified that the issues involving the role of parameter WFBETCEL in sensitivity analyses have been resolved.

Figure 12-1. Combined Mean CCDFs for Components of Total Normalized Releases for All PABC-2009 Replicates

(Source: Clayton et al. 2010, Figure 6-7)
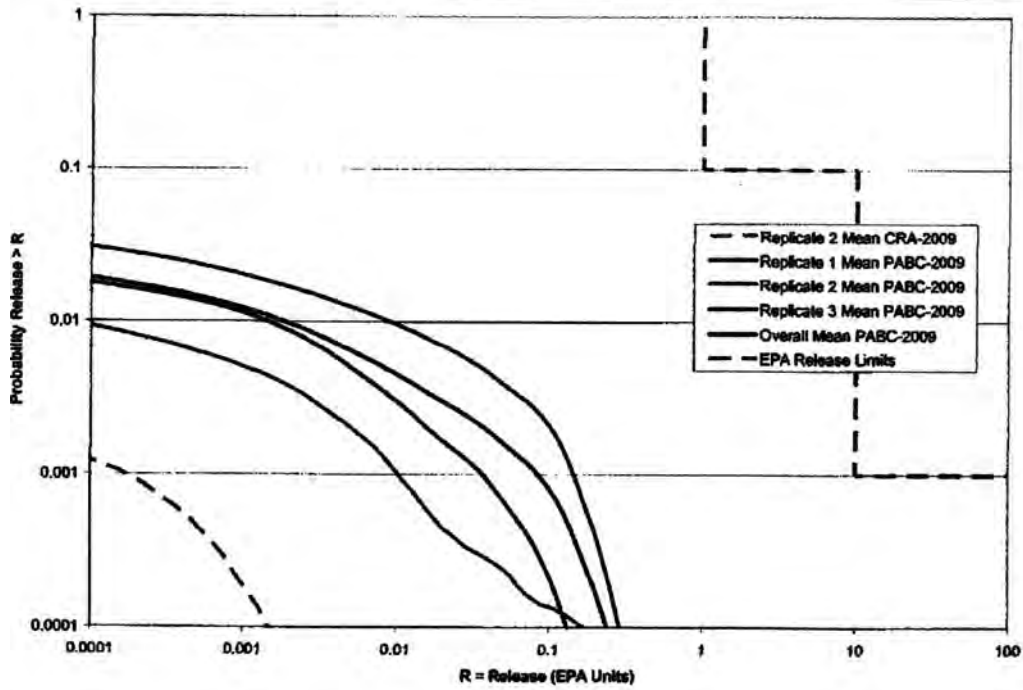
**Figure 12-2.   PABC-2009 and CRA-2009 Replicate Mean CCDFs for
Normalized Culebra Transport Releases**

Note that PABC-2004 and CRA-2009 results are virtuall identical. (Source: Camphouse 2010b, Figure 3-27)

Figure 12-3.   Overall Mean CCDFs for Total Normalized Releases: CRA-2009 PA and CRA-2004 PABC

(DOE 2009, Figure PA-1)

Figure 12-4.   Overall Mean CCDFs for Total Normalized Releases for CRA-2009 PA and PABC-2009

(Clayton et al. 2010, Figure 6-8).

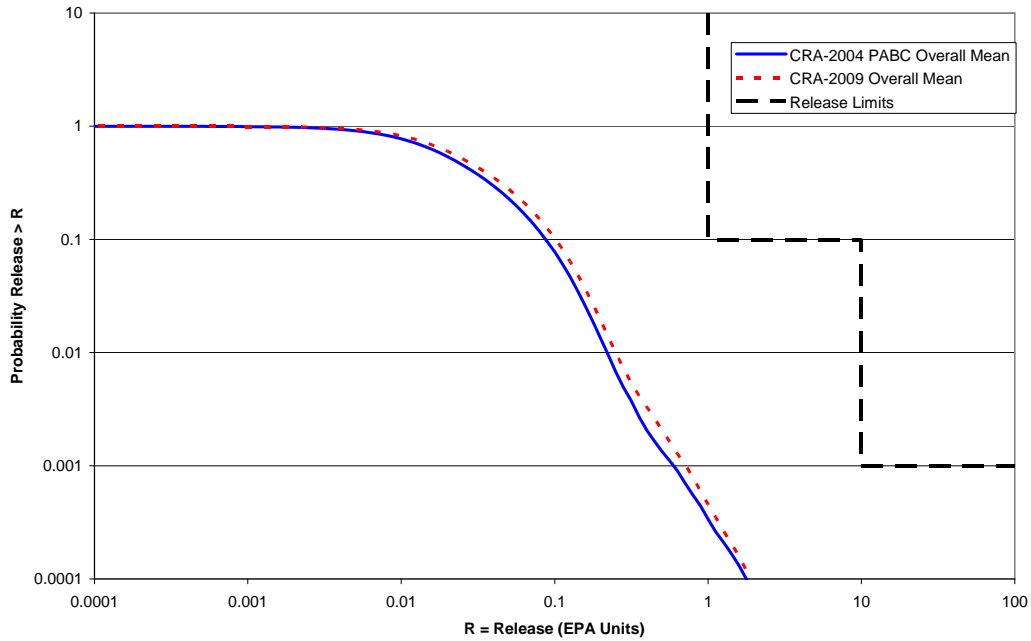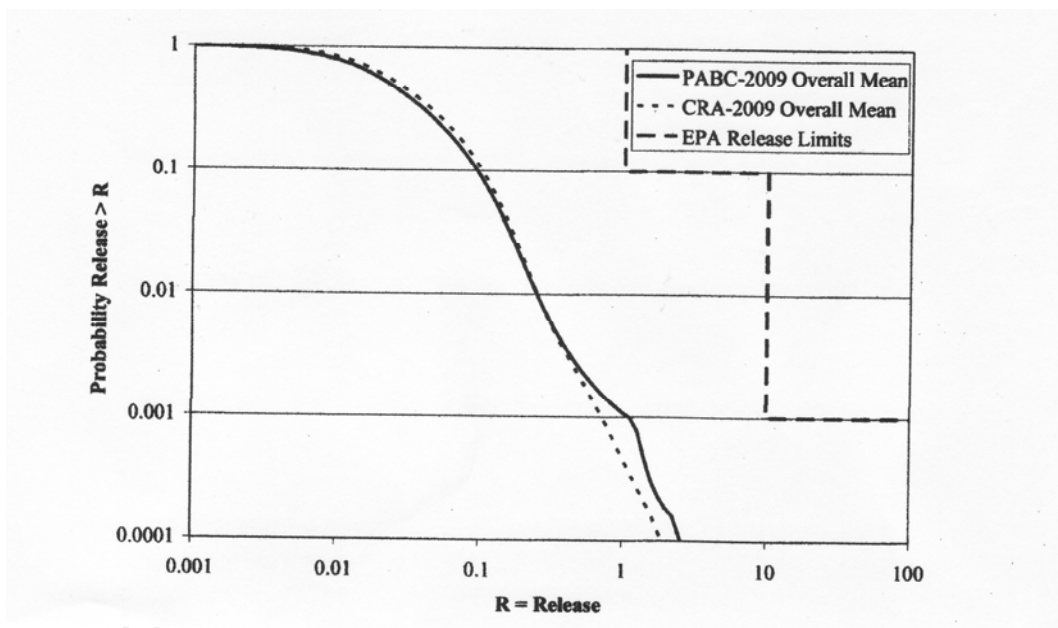**Table 12-3.   Stepwise Rank Regression Analysis – Comparison of PABC-2004, CRA-2009 PA, and PABC-2009 Results**

Step[a]	Expected Normalized Release								
	PABC-2004			CRA-2009 Replicate 1			PABC-2009 Replicate 1		
	Parameter[b]	SRRC[c]	$R^{2[d]}$	Parameter[b]	SRRC[c]	$R^{2[d]}$	Parameter[b]	SRRC[c]	$R^{2[d]}$
1	WTAUFAIL	-0.94	0.88	WTAUFAIL	-0.90	0.81	WTAUFAIL	-0.88	0.76
2	WSOLVAR3	0.14	0.91	WSOLVAR3	0.17	0.84	WSOLVAR3	0.17	0.79
3	DOMEGA	0.10	0.92	WFBETCEL	-0.11	0.85	WFBETCEL	-0.14	0.81
4	WFBETCEL	-0.09	0.93	DOMEGA	0.10	0.86	BPINTPRS	0.12	0.83
5	BPINTPRS	0.08	0.93	SHURGAS	-0.08	0.87	BPPROB	0.13	0.85
6	BPPROB	0.07	0.94	BPINTPRS	0.07	0.88	SHURGAS	-0.10	0.85
7	SHURGAS	-0.06	0.94	BPPROB	0.08	0.89	CTRAN	0.09	0.86
8	SHLPRM2	0.06	0.95	CTRAN	0.08	0.89	DOMEGA	0.08	.087

PABC-2004 results from Leigh et al. 2005a, Table 7-2

CRA-2009 and PABC-2009 results from Kirchner 2010b Table 4.

(a)   Steps in stepwise regression analysis

(b)   Parameters listed in order of selection in regression analysis

(c)   Standardized Rank Regression Coefficient in final regression model

(d)   Cumulative R^2 value with entry of each variable into regression model

13.0 SUMMARY AND CONCLUSIONS

In its July 16, 2009, letter (Cotsworth 2009a) EPA advised DOE that a revised PA was required for recertification, replacing the PA included in the 2009 Compliance Recertification Application submitted by DOE. As stated by Cotsworth:

> *EPA believes it is necessary to perform a new performance assessment to capture changes since the last recertification, as was done in 2004. The Agency also believes that even though our CRA-2009 review is not yet complete, it is necessary to notify DOE of this need as soon as possible. In particular, changes in the waste inventory since the 2006 performance assessment baseline calculations must be addressed. Specifically, the organic chemical materials have, in some cases, significantly increased and their impact (e.g., solubilities, etc.) needs to be incorporated into the CRA-2009 performance assessment calculations to verify continued compliance with our regulations. As in the past, DOE is expected to find and correct errors in the previous performance assessments. DOE is also expected to include the new Culebra hydrology model peer reviewed in 2008 and to include the most recent parameters, such as the updated drilling rate and revised borehole plugging patterns.*

EPA's review as to the whether the requested changes were appropriately implemented in the revised PA (the PABC-2009) is summarized below.

Waste Inventory

As described in Section 3, the inventory used in the CRA-2009 PA was replaced by the year ending inventory for 2007 (ATWIR 2008, PAIR 2008), which was the most recent inventory available at the time of the EPA request. EPA reviewed the documentation used to develop this inventory and the computer codes used to manipulate the inventory data into formats required for PA. EPA also determined that the correct inventory-related parameters had been introduced into the PABC-2009. EPA is satisfied that the requested changes to the waste inventory have been properly accomplished.

Organic Ligands

DOE used the most recent inventory data (Crawford et al. 2009) and the most recent estimate of the minimum brine volume necessary for DBR (Clayton 2008) to calculate organic ligand concentrations for the PABC09 (Table 7-2, Brush and Xiong 2009). Because the most recent inventory data for organic ligands were incorporated in the actinide solubility calculations, the effects of the updated inventory on the dissolved actinide source term were accounted for in the PABC09 calculations. The aqueous speciation and solubility calculations were carried out both with and without the predicted organic ligand concentrations. The results obtained with organic ligands were used to determine dissolved actinide source term concentrations for the PABC09. EPA has concluded that the approach used in the PABC09 involving use of the revised minimum brine volume and the most recent information on concentrations of organic ligands to calculate actinide solubilities is scientifically-sound and appropriate for PA.

Culebra Hydrology Model

The Culebra hydrology conceptual model describes the overall hydrogeologic framework of the Culebra Dolomite Member of the Rustler Formation in the vicinity of the WIPP site. The Culebra stratigraphic unit is the most significant potential groundwater transport pathway for radionuclides released from the WIPP repository. Although the original conceptual model was inadequate, this was of little consequence, because release of radionuclides through the Culebra was very limited.

Howver, in response to concerns that the original conceptual model for Culebra hydrogeology developed for the CCA did not establish a strong correlation between the conceptual model and the numerical model used in PA, DOE revised the Culebra hydrology model to establish a stronger link between the Culebra hydrogeology and the numerical hydrogeologic model. As part of this process, the DOE also sought to improve the ability of the model to reproduce the observed hydrologic behavior of the Culebra with respect to fluid flow.

Once the DOE completed their revision to the Culebra hydrology conceptual model (identified as the RCHCM), it was subjected to independent peer review (Burgess et al. 2008). The Panel reviewed sedimentological, geochemical, hydrologic, numerical simulations and geostatistical information that the DOE integrated to form the conceptual model. The Panel also reviewed the method by which that information was used to develop calibrated T-fields. In its assessment of the validity of conclusions reached through use of the conceptual model, the Peer Panel made the following statement:

> *The Panel believes that the conclusions in the RCHCM from the integration of geology and hydrology are valid, and can be used to develop T-fields for incorporation in the PA.*

As discussed in EPA 2008, the Agency agreed with the Panel's conclusion on the basis of the rationale presented in the Panel's report, and also on the basis of the demonstrated improvement in the ability of the RCHCM to be calibrated to measured heads and transient field test results over that of the previous Culebra flow model. EPA is satisfied that the current Culebra hydrology model is appropriate for use in PA and was correctly implemented in PABC-2009.

Drilling Parameters

The drilling rate and the borehole plugging patterm probabilities were updated based on the most recent Delaware Basin Annual Monitoring Report for the period ending August 31, 2008 (EPA 2010f). The revised parameters were correctly introduced into the PAPDB.

Parameters

Many of the modifications required for the PABC-2009 necessitated changes to parameters used in modeling PA. As described in Section 5, EPA validated all parameter changes made from the CR-2009 PA to the PABC-2009.

13.1 CONCLUSION

Based on the information presented here, EPA is satisfied that the revised PA (PABC-2009) contains all of changes requested by the Agency. These changes are transparent, traceable against prior PAs, consistent with EPA direction, and have been properly implemented. The PABC-2009 results described in Section 12 show that the WIPP continues to comply with the containment requirements of 40 CFR 191.13.

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