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**TECHNICAL SUPPORT DOCUMENT:  
OVERVIEW OF MAJOR PERFORMANCE ASSESSMENT ISSUES**

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## Technical Support Document: Overview of Major Performance Assessment Issues

### 1.0 Introduction

The Department of Energy's (DOE) Compliance Certification Application (CCA) for the Waste Isolation Pilot Plant (WIPP) is a complex document that endeavors to show compliance with 40 CFR parts 191 and 194. Of these two regulations, 40 CFR part 191.13 and its implementation criteria in sections of 40 CFR part 194 are perhaps the most important portions that directly affect the potential performance of WIPP. Other criteria are important inasmuch as they contribute to the process of generating the inputs to the performance assessment (PA), or are subsets of the PA, as is the case with the individual and ground-water protection requirements. §191.13 identifies the general performance standard to which the WIPP must adhere and the containment requirement sections of 40 CFR 194 provide specific criteria that the WIPP PA must consider. For example, §194.32 identifies the scope of activities that DOE must consider in its WIPP PA. In addition, the containment requirements section of 40 CFR part 194 specify general requirements that DOE must follow and document in the CCA. §194.23 requires DOE to document the conceptual model and computer code development process. §194.24 requires DOE to, among other things, identify the waste characteristics that may affect performance of the WIPP disposal system and include them into the PA calculations.

Documentation of EPA's review of the DOE's WIPP CCA is provided in specific Compliance Application Review Documents (CARDs) and associated technical support documents (TSDs). This PA technical support document is intended to summarize PA related issues that are addressed in multiple review documents (CARDs and TSDs). Because of the range of complexity of PA issues, the intent of this document is to address issues that affect or could potentially impact the results. The major topics to be discussed in this document are:

- Overview of Important Geologic Issues at WIPP.

Site characterization provides the basis for the conceptual models, the screening of features, events and processes, and the development of many parameters. An introduction to the major characteristics of the site will be provided to lay a foundation for the remainder of the topics discussed. For additional details on this topic, see the Technical Support Document for Section 194.14: Content of Compliance Certification Application (Docket A-93-02, Item V-B-3).

- Performance Assessment Process.

The PA process consists of characterizing the site, the development of conceptual models and the implementation of the conceptual model in computer codes using mathematical and numerical models. This section provides an overview of the process and a brief summary of EPA's review of DOE's computer code development and selected computer codes.

The PA computer codes consist of those computer codes that perform the calculations that model processes, and computer codes that support the PA computer codes. As is the case with the conceptual models, some PA computer codes affect the results more than others. EPA's review of the computer codes raised questions (e.g., mass balance in the code SECOTP2D) about some of the codes. This, in turn, raised questions about the CCA results and their adequacy. DOE identified and corrected specific problems with the computer codes.

DOE identified 24 major conceptual models that use site characterization information to capture those elements of the site that are believed to affect the performance of WIPP. These concepts of the site are quantified into equations and parameter inputs which are solved using a series of computer codes. DOE's evaluation work, previous PAs and the CCA have shown that some of these conceptual models are more important than others in determining how well the WIPP can contain radionuclides. For additional details see the Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6, section 1).

- Important Modeling Issues

DOE identified a number of site features (e.g., stratigraphy), potential events (e.g., drilling) and potential processes (e.g., groundwater flow in the Culebra dolomite or gas generation due to corrosion and microbial processes). In its site characterization process, DOE also identified potential features, events and processes (FEPs) that are unlikely to occur (e.g., meteorite impacts) or would not substantially affect the ability of WIPP to contain radionuclides (e.g., shallow drilling and karst). For additional details see the Technical Support Document for Section 194.32: Scope of Performance Assessments (Docket A-93-02, Item V-B-21, section 4).

- EPA Mandated Performance Assessment Verification Test (PAVT).

As stated above EPA's review identified concerns with some parameter values and computer codes. The public also raised similar concerns. Since there were changes to the parameter values and some of the computer codes, EPA directed DOE to conduct additional PA calculations in a Performance Assessment Verification Test (PAVT). EPA's goal was to verify that the cumulative impact of the changes did not significantly change the releases predicted by the CCA PA. The results of the PAVT were well below the containment requirements of §191.13. This indicated that the EPA directed changes to the parameters and the changes DOE made to the computer codes were not significant. The PAVT results thus verify that the CCA calculations are acceptable as the bases for EPA's compliance determination decision. (Also see the reports at Docket A-93-02, Items II-G-26 and II-G-28, prepared by DOE on PAVT results.)

## 2.0 Overview of Important Geologic Issues at WIPP

The WIPP is located in the Delaware Basin of New Mexico and Texas and is approximately 26 miles southeast of Carlsbad, New Mexico. The Delaware Basin contains thick sedimentary deposits (15,000 - 20,000 feet), including the Salado Formation, the rock formation in which DOE plans to place radioactive waste. Since the Salado Formation was deposited about 200-250 million years ago, the Delaware Basin has been a stable, undisturbed geologic region as reflected by the nearly horizontal sedimentary rocks of the Delaware Basin. Major events such as large scale earthquakes or volcanic activity have been reviewed and screened out as very low probability events over the regulatory time frame of 10,000 years.

While there are numerous geologic formations underneath the WIPP site, DOE identified that the formation immediately below the repository horizon and upward to the surface are the primary geologic units of concern. They are (from below the repository to the surface):

- ◆ Castile Formation-- consisting of anhydrite and halite with a few pressurized brine pockets found locally near the WIPP site.
- ◆ Salado Formation-- consisting primarily of halite with some anhydrite interbeds and accessory minerals and approximately 2,000 feet (600 meters) thick.
- ◆ Rustler Formation-- containing salt, anhydrite, clastics, and carbonates (primarily dolomite), with the Culebra member of the Rustler as the unit of most interest since it is the most transmissive unit above the Salado.
- ◆ Dewey Lake Red Beds Formation (Dewey Lake) -- consisting of sandstone, siltstone and silty claystone.

Geologic formations below these were included in the screening of features, events, and processes, but were not included in PA calculations because they had no impact on potential radionuclide releases.

DOE indicated that the major geologic process in the vicinity of WIPP is dissolution of the halite. To the west, the slight (1°) dip in the disposal system geologic units has exposed the Salado to dissolution processes; however, DOE estimated that this lateral dissolution front will not reach the WIPP site for hundreds of thousands of years. DOE indicated that while deep dissolution has occurred in the Delaware Basin, the process of deep dissolution would not occur at such a rate at the WIPP site that it would impact the containment capabilities of the WIPP during the regulatory time period. Near-surface dissolution of evaporitic rocks (e.g., gypsum) has created near-surface karst topography west of the WIPP site, but karst processes do not appear to have affected the rocks within the WIPP site itself near the level of the waste.

Karst features such as Nash Draw have formed via shallow (surface down) dissolution in the WIPP area. DOE indicated that the development of karst features near and above the WIPP has been the subject of considerable study, and concluded that development of near surface karst

does not pose a threat to the containment capabilities of the disposal system. EPA examined the information presented within the CCA and acknowledges that karst terrain is present in the vicinity of the WIPP site boundary (Chapter 2, Sections 2.1.3.4 and Chapter 2.1.6.2, pp. 2-87 to 2-93, and Appendix DEF 3.3). Nash Draw, which is approximately one mile west of the WIPP site, is attributed to shallow dissolution and contains karst features. Available data suggest that dissolution-related features occur in the WIPP area (e.g., WIPP-33), but these features are not associated with any identified preferential groundwater flow paths or anomalies in the WIPP Land Withdrawal Area (LWA). Karst terrain typically exhibits cavernous flow, blind streams, and potential for channel development that would enhance fluid and contaminant migration. Data from SNL tracer tests in the LWA do not indicate the presence of anomalous cavernous-type flow; for example, the interpretation of the H-2 hydropad, located just west of the waste panel area, is one of single (matrix) porosity, not channeling (CCA Reference 343). Additional information on karst, including EPA's response to comments about karst and shallow dissolution can be found in CARD 14 (A-93-02, V-B-2).

DOE indicated that some of the geologic formations below the repository area contain oil and gas, resources that are currently being exploited in the Delaware Basin. In addition, potash is found within the Salado; however, the waste area lies below an area where there are no economically minable reserves. Refer to Section 2.3.1 (p. 2-147) of the CCA for more information. According to DOE analysis, most of the water in the vicinity of WIPP is highly saline, with the closest dependable potable aquifer associated with the Capitan Reef surrounding the Basin. In §194.33 EPA directs DOE to use the current drilling rate as an estimate of the future drilling rate. At the current deep drilling rate of 46.8 boreholes per year per square kilometer, it is expected that WIPP (waste area of 0.126 square kilometers) could average five drilling intrusions in the 10,000 year computer simulation realizations.

The potential pathways for radionuclide transport are the Salado anhydrite interbeds and the Culebra dolomite member of the Rustler Formation. While more permeable than the halite, the Salado anhydrite interbeds are still very impermeable ( $\sim 10^{-19}$  m<sup>2</sup> permeability for the anhydrite versus  $\sim 10^{-21}$  m<sup>2</sup> permeability of the halite). The Culebra is conceptualized as a  $\sim 8$  meter thick, dual-porosity dolomite, in which flow and transport are believed to be confined in the lower half of the 8 meter thickness. Due to the very low permeability of the Salado halite, a borehole through the waste is necessary before radionuclides can access the Culebra.

### 3.0 Performance Assessment Process

As stated in §191.12, "Performance assessment means an analysis that: (1) identifies the processes and events that might affect the disposal system; (2) examines the effects of these processes and events on the performance of the disposal system; and (3) estimates the cumulative releases of radionuclides, considering the associated uncertainties, caused by all significant processes and events. These estimates shall be incorporated into an overall probability distribution of cumulative release to the extent practicable." The "overall probability distribution of cumulative release" refers to complementary cumulative distribution functions or CCDFs. The use of CCDFs for PA is required in §194.34(a).

DOE also has to conduct a compliance assessment as required in 40 CFR part 194.55. Compliance assessment is essentially a PA of the undisturbed case and has separate requirements for reporting the results (i.e., CCDFs need not be used for compliance assessments). However, the WIPP compliance assessment is a subset of the PA. Most of the discussion for PA also applies to compliance assessment. Thus, compliance assessments will not be singled out for discussion here. (See Technical Support Document for Section 194.55: Compliance Assessment Statistics (Docket A-93-02, Item V-B-26.)

The results of the WIPP PA calculations form the basis for understanding a disposal system's potential behavior and identify whether the disposal system can comply with the containment requirements at §191.13. The development of a PA involves numerous components, including site characterization, conceptual models, parameters for use in computer codes, and computer codes (mathematical and numerical models). The results presented in CCDFs provide the basis for determining compliance.

Section 194.23 sets forth specific requirements for the models and the computer codes used to calculate the results of PAs. In order for these calculations to be reliable, DOE must properly design and implement the computer codes used in the PA. Design of computer codes is preceded by and concurrent with characterization of the site and the development of conceptual models. Conceptual models consider the design of the repository and the features, events, processes, and scenarios that may occur at the WIPP which could affect the containment or release of radionuclides. In order for the final computer codes to obtain realistic solutions, the underlying conceptual models must be sound and the parameters used by the computer codes need to be appropriate for their use.

### 3.1 Site Characterization

As noted in Figure 1 of this technical support document, modeling results are the culmination of many elements, including the characteristics of the site and regulatory requirements. The characteristics of the site largely establish which features, events, and processes (FEPs) could be expected to occur in or around the disposal system. FEP evaluation is based on the results or characteristics learned during site characterization activities, results of facility design, and the results of waste characterization activities. Site characterization activities provide information on the geologic and hydrogeologic characteristics of the disposal site, such as the identification of potential radionuclide pathways, including the hydrology of the transmissive units (i.e., the Culebra member of the Rustler formation) and the mechanical nature of the Salado halite (i.e., the ability to move or creep under pressure). Facility design is based on the structural requirements of the underground mine, such as small disposal rooms with large intervening support pillars, and the expected disposal operation methods, such as an expected 30 to 40 year operation life. The characteristics of the waste and the interaction of the waste with site features, events, or processes may or may not impact the long-term confinement of the waste placed into the disposal system. Waste characterization activities include an evaluation of the chemical interaction characteristics of the waste components and the long-term degradation of waste components under conditions expected to occur at the site. Information about site

characteristics, facility design, and waste characterization are used to make conceptual models that are important to the performance of the disposal system.

### 3.2 Conceptual Model Development

FEPs selected during the FEP evaluation process and regulatory requirements (such as Section 194 mining requirements and human intrusion requirements) are developed into different conceptual models that, often in a simplified manner, emulate the important characteristics of the disposal system. It is impossible to model every detail of any system, therefore, it is necessary to create simplifications that adequately address the important features, events, processes that could occur. DOE has created conceptual models that attempt to capture the elements that should be modeled as well as how they should be modeled. Table 1 of this technical support document list the twenty four conceptual models developed for the WIPP CCA PA. The most important of the conceptual models include human intrusion characteristics and resulting types of processes, such as cutting and cavings, spallings, and direct brine release. These are specifically discussed in Section 4 of this report.

Once these conceptual models are developed, mathematical models are then derived to quantify the conceptualization in a form that can be evaluated using computer codes that include appropriate numerical solution methods. Examples include the governing equations of flow and transport of brine and gas in the disposal room. These equations express mass balance, initial conditions, and boundary conditions that model the dynamic characteristics of the disposal environment. These mathematical expressions of the conceptual models are captured in equations and then incorporated into computer programs which actually “model” the disposal system, the waste disposed, and the surrounding environs in order to project potential radionuclide transport.

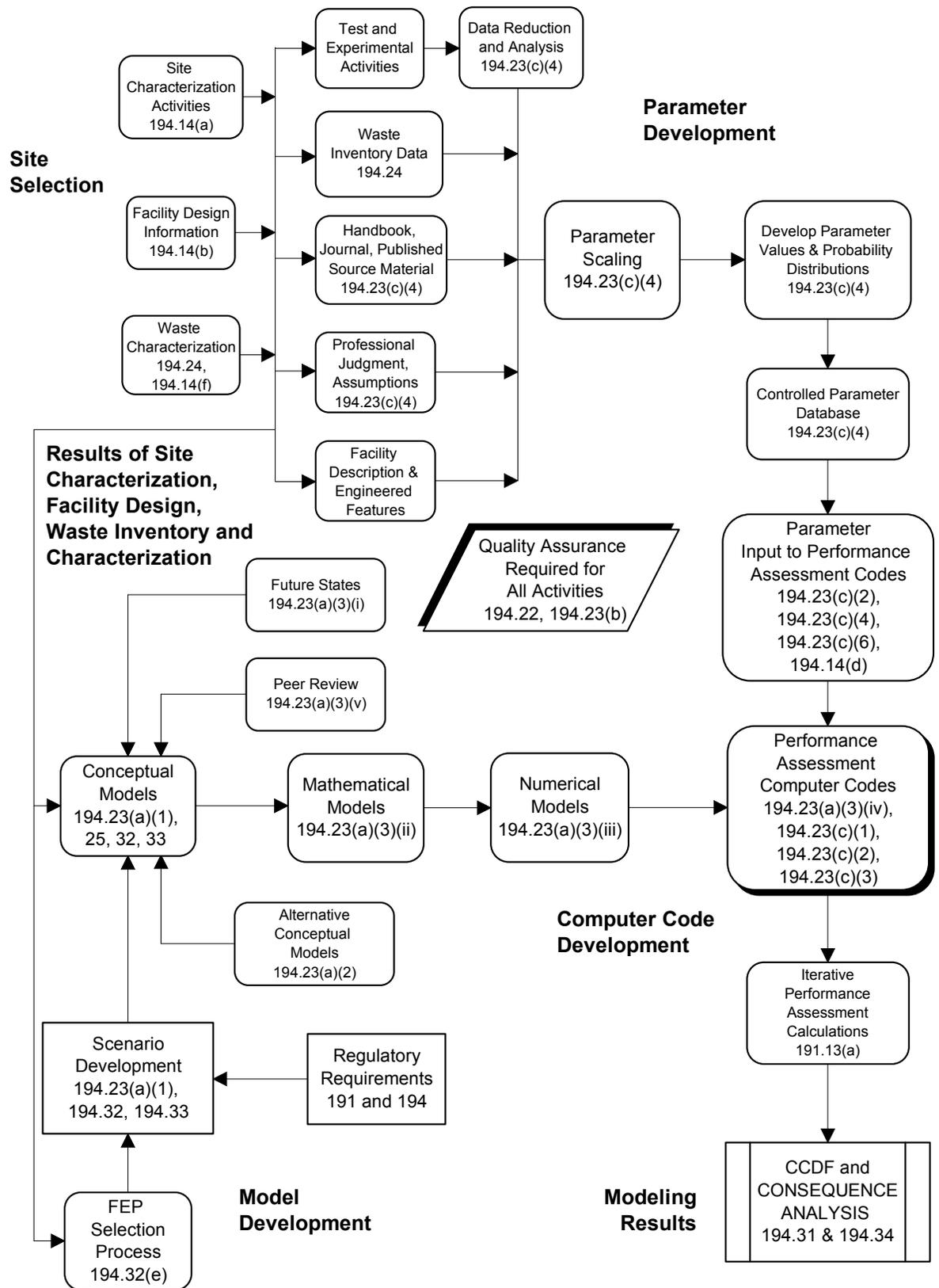
EPA reviewed each of the 24 conceptual models included in the CCA using information contained in the CCA, supplementary peer review panel reports, and supplementary information provided to EPA by DOE in response to specific EPA comments. EPA agreed with the Conceptual Model Peer Review Panel (CMPRP) (Docket A-93-02, Item II-G-22) that all models except the spallings model were adequate for use in the PA calculations. The CMPRP found that the original PA spallings model only modeled the ‘end state of the waste’ and did not fully model all potential mechanisms that may drive pressure driven solid releases. However, the peer review panel also found in its Third Supplementary Peer Review Report (Docket A-93-02, Item II-G-22, Section 4.0 Summary, p. 17) that the results from the spallings model are reasonable and that they may even overestimate releases. EPA agreed with this finding because DOE showed in its additional spallings modeling that the release of solid waste predicted by the PA spalling model overestimates releases by ten times or more.

EPA’s review found that the CCA and supplementary information contained a complete and accurate description of each of the conceptual models used and that documentation of the conceptual models adequately discussed site characteristics and processes active at the site. EPA determined that the conceptual models adequately represent those characteristics, processes, and attributes of the WIPP disposal system affecting its performance, and that the conceptual models

consider both natural and engineered barriers. EPA found that DOE considered conceptual models that adequately described the future characteristics of the disposal system and its environs. The conceptual models reasonably described the expected performance of the disposal system and incorporated reasonable simplifying assumptions of the behavior of the disposal system.

### 3.3 Computer Code Development

As noted in Figure 1, the PA is actually captured in the form of modeling results from computer codes. These results, in the form of CCDFs, are used in determining compliance with the containment requirement at §191.13. A series of computer codes were developed because of the massive complexity of the disposal system and its environs. The mathematical equations that are the final expression of the conceptual models are programmed into FORTRAN computer codes that are used to “model” the disposal system. For example the BRAGFLO computer codes includes the mathematical equations for gas generation, shafts and shaft seals, Castile brine reservoir, exploration boreholes, disturbed rock zone, and Salado interbeds to name a few. The SECOFL2D and SECOTP2D computer codes include climate change, transport of dissolved actinides in the Culebra, and transport of colloidal actinides in the Culebra to name a few.



**Figure 1** Generalized Performance Assessment Development Flowchart

Performance assessment computer codes are generally executed in this order: BRAGFLO is used to model the longer term history of the disposal system, PANEL and NUTS are used to model the transport of actinides dissolved in brine, and SECOFL2D and SECOTP2D are used to model the flow and transport of actinides in the Culebra unit of the Rustler formation. The short-term release of brine flowing up a borehole is modeled in the direct brine release setup of the BRAGFLO computer code, called BRAGFLO\_DBR; then PANEL is used to model actinide dissolution in brine and movement to the surface in the case of multiple intrusions into one panel. CUTTINGS\_S is used to model the short term amount of radioactive material removed by cutting and caving processes and those releases due to spalling processes. The releases predicted by all of these release mechanisms are combined in the CCDFGF computer code to predict the cumulative releases of the modeling system.

Table 1

WIPP Conceptual Models Used in CCA

<b>Model</b>	<b>Component</b>
1 Disposal System Geometry	Salado F/T <sup>1</sup>
2 Culebra Hydrogeology	Non-Salado F/T
3 Repository Fluid Flow	Salado F/T
4 Salado	Salado F/T
5 Impure Halite	Salado F/T
6 Salado Interbeds	Salado F/T
7 Disturbed Rock Zone	Salado F/T
8 Actinide Transport in the Salado	Salado F/T
9 Units Above the Salado	Non-Salado F/T
10 Transport of Dissolved Actinides in the Culebra	Non-Salado F/T
11 Transport of Colloidal Actinides in the Culebra	Non-Salado F/T
12 Exploration Boreholes	Human intrusion
13 Cuttings and Cavings	Human intrusion
14 Spallings	Human intrusion
15 Direct Brine Release	Human intrusion
16 Castile and Brine Reservoir	Human intrusion
17 Multiple Intrusions	Human intrusion
18 Climate Change	Non-Salado F/T
19 Creep Disposal	Salado F/T
20 Shafts and Shaft Seals	Salado F/T
21 Gas Generation	Salado F/T
22 Chemical Conditions	Salado F/T
23 Dissolved Actinide Source Term	Salado F/T
24 Colloidal Actinide Source Term	Salado F/T

<sup>1</sup>F/T - flow and transport.

3.4 Selected Performance Assessment Computer Codes

Based on the conceptual model derivation DOE developed the following computer codes: PANEL, BRAGFLO, NUTS, FMT, SANTOS, BRAGFLO\_DBR, GRASP\_INV, SECOFL2D, SECOTP2D, CCDFGF, and CUTTINGS\_S. These are the codes DOE used to model the behavior of the repository and its surroundings and to compute the results of the PA calculations. PANEL, BRAGFLO, NUTS, FMT, and SANTOS implement the conceptual models for predicting future characteristics of the waste repository. These five codes simulate the following effects, respectively: concentrations of radioactive waste in brine within the waste-containing panels in the repository; flow of brine and gas in the repository; solubility and transport of radionuclides released from the repository; solubility of radionuclides in the repository; and collapse of the repository through salt creep closure of the Salado. The computer code BRAGFLO\_DBR describes waste dissolution in brine and transport of the contaminated brine through direct brine releases. The three computer codes GRASP\_INV, SECOFL2D, and SECOTP2D describe flow and transport of waste-laden brine in the Culebra dolomite. The computer code CUTTINGS\_S models releases of radioactive waste upon intrusion of a drill bit into the repository. The computer code CCDFGF computes complementary cumulative distribution functions (CCDFs) for the results of PA.

EPA encountered problems with the governing equations of the mathematical models and the representation of the boundary conditions in the codes CUTTINGS\_S, SECOFL2D, SECOTP2D, NUTS and BRAGFLO (see Technical Support Document for Section 194.23: Models and Computer Codes, Section 4.0, Docket A-93-02, Item V-B-6). EPA specified that the equations in the code be corrected and that the changes to the code be documented.

EPA's review identified stability concerns related to the following codes: CUTTINGS\_S, SECOFL2D, SECOTP2D, and NUTS (see Technical Support Document for Section 194.23: Models and Computer Codes, Section 5.0, Docket A-93-02, Item V-B-6). In the case of the NUTS and SECOTP2D codes, DOE was able to make minor changes to the codes to correct their stability problems. EPA's concerns regarding potential stability problems with CUTTINGS\_S and SECOFL2D were alleviated after DOE provided results from further stability and code verification testing that showed these problems had been corrected. DOE satisfactorily resolved all EPA concerns regarding code stability issues.

EPA identified issues related to coding errors for the following codes: SECOFL2D, SECOTP2D, and NUTS (see Technical Support Document for Section 194.23: Models and Computer Codes, Section 6.0, Docket A-93-02, Item V-B-6). To address these concerns, EPA requested that DOE perform a number of additional analyses. In the process of responding to EPA's concerns, DOE discovered, rectified and documented several minor coding errors. Results from an impact analysis by DOE indicated that the coding errors would have had very little impact on the WIPP's compliance with the disposal regulations. These issues were resolved to EPA's satisfaction.

### 3.5 Parameter Development

Parameters are numerical values or ranges of numerical values used to describe different physical and chemical aspects of the repository, the geology and geometry of the area surrounding the WIPP, and possible scenarios for human intrusion (see Technical Support Document for Section 194.23: Parameter Report, Docket A-93-02, Item V-B-12). Some parameter values are well-established physical constants, such as the Universal Gas Constant or atomic masses of radionuclides. Parameters also can be physical, chemical or geologic characteristics that DOE establishes by experimentation. DOE has also used parameters that consider the effects of human intrusion, such as the diameter of a drill bit used to drill a borehole that might penetrate the repository.

Figure 1 notes that parameters are placed in a controlled database to provide values needed for the PA computer codes. Parameters, such as waste inventory values, waste solubility and retardation characteristics, rock units characteristics, and site related activities which include mining and oil and gas drilling, are used as input values to the PA computer programs. These parameters values originated from multiple sources, which include laboratory and field testing and experimental activities; waste characterization activities such as waste inventory estimates; scientific handbooks, journals, other published source materials; professional judgement used to interpret information; and facility design description and engineering features of the disposal system. Parameters may have to be scaled to account for expected future conditions or expected future characteristics of the disposal system. Finally the developed parameters are placed in the controlled database so the PA computer programs can access the parameter values when needed during the calculations.

EPA reviewed the CCA, parameter documentation and record packages for approximately 1,600 parameters used as input values to the CCA PA calculations. EPA further reviewed parameters record packages and documentation in detail for 465 parameters important to performance of the disposal system. EPA selected parameters to review in depth based on the following criteria: parameters that were likely to contribute significantly to releases or seemed to be poorly justified; parameters that control various functions of the CCA PA computer codes that were likely to be important to calculations of releases and important to compliance with the containment requirements of §191.13; and other parameters the Agency used to evaluate the overall quality of Sandia National Laboratory's (SNL) documentation traceability. The Agency examined DOE's parameter documentation to see if the following elements were present: detailed listings of code input parameters and the parameters that were sampled; codes in which the parameters were used and the computer code names of the sampled parameters; descriptions of the sources of data; descriptions of the parameters, data collection procedures, data reduction and analysis, and code input parameter development; discussions of the linkage between input parameter information and data used to develop the input information; discussions of the importance of the sampled parameters relative to final calculations of releases, correlations among sampled parameters, and how these are addressed in PA; a listing of the sources of data used to establish parameters; and data reduction methodologies used for CCA PA parameters used in the calculations, including an explanation of quality assurance activities. EPA's detailed review of the parameters used in the CCA PA calculations can be found in the Technical Support Document for Section 194.23: Parameter Report, Docket A-93-02, Item V-B-12; the Technical Support Document for Section for 194.23: Sensitivity Analysis Report, Docket A-93-02, Item V-

B-13; and the Technical Support Document for Section 194.23: Parameter Justification Report, Docket A-93-02, Item V-B-14.

After its initial review, EPA found that DOE did have a great deal of documentation available in the SNL Records Center supporting most of the parameters used in the CCA PA. However, EPA had some concerns about the completeness of the list of CCA PA parameters, the description and justification that support the development of some code input parameters, and the traceability of data reduction and analysis of parameter-related records. EPA did not agree with the technical justification of some parameter values and probability distributions. EPA did not find adequate documentation to support one of DOE's professional judgement parameters, the particle size diameter value. Other parameters such as professional judgement parameters and some parameters that were used in DOE's 1992 PA calculations were found to have adequate documentation to support the value used in the CCA PA calculations.

During its review process, EPA found that the following types of documentation were necessary to improve DOE's records: a comprehensive database of all parameters used in the WIPP CCA PA, a database of all parameters based on experimental data, "roadmaps" that document and link CCA PA parameters to their sources, complete record packages in the SNL Record Center, background documentation on the development of those parameters that were originally used in DOE's 1992 PA calculations and again were used in the CCA PA calculations, and adequate explanations of why the 149 professional judgement parameters in the comprehensive parameter database did not need expert elicitation. DOE provided all of these pieces of documentation, primarily by improving the quality of the records stored in the SNL WIPP Records Center. EPA did not accept the professional judgement parameter of waste particle size, and the Agency required DOE to use the process of expert elicitation to develop the value for this parameter. (see Technical Support Document for Section 194.23: Models and Computer Codes, Section 7.0, Docket A-93-02, Item V-B-6 and CARD 26-Expert Judgment, Docket A-93-02, Item, V-B-2.) After subsequent review and evaluation of the SNL WIPP Record Center records and after completion of expert elicitation, EPA was satisfied with the additional documentation provided by DOE for these areas of concern.

EPA requested further documentation from DOE, expressing concern about information supporting 58 parameters. EPA divided these parameters into those parameters lacking supporting evidence, those parameters that have supporting records for values other than those selected by DOE, and those parameters that are not explicitly supported by the relevant data or information. DOE provided additional information supporting some of the parameters of concern to EPA. EPA also performed its own sensitivity analyses upon the parameters to determine if changes to some parameters have a significant impact upon the final computer calculations. (See Technical Support Document for Section 23: Sensitivity Analysis Report (Docket A-93-02, Item V-B-13.) The Agency's concerns about thirty-four of these parameters were resolved, either by DOE's submission of additional documentation or by the results of sensitivity analyses conducted by EPA that indicated that changes to certain parameter values would not significantly impact final computer calculations.

Upon subsequent review and evaluation, EPA determined that DOE, after additional work and improvement of records in the SNL Record Center, adequately provided a detailed listing of the code input parameters; listed sampled input parameters; provided a description of parameters and the codes in which they are used; discussed parameter correlations and parameters important to releases; described data collection procedures, sources of data, data reduction and analysis; and described code input parameter development, including an explanation of quality assurance activities.

EPA required DOE to perform additional calculations in a PAVT in order to verify that the cumulative impact of all necessary corrections to input parameters, conceptual models, and computer codes used in PA was not significant enough to necessitate a new PA. EPA directed DOE to incorporate modified values or distributions for twenty-four parameters in the PAVT. The PAVT showed that the calculated releases may increase by up to three times from those in the original CCA PA values for the mean calculated releases and that the WIPP is still an order of magnitude below the Agency-mandated containment requirements in §191.13. The results of the PAVT required by EPA demonstrated that the combined effect of all the required changes does not significantly alter the predicted performance of the repository.

### 3.6 Modeling Results

In order to evaluate the many scenarios conceptualized for the disposal system at WIPP iterative, multiple calculations, are done. During each stage of modeling calculations the computer codes report results, prints out, of their calculations. For example, during operation BRAGFLO prints out the results of each step of its calculations, such as its operational efficiency and important parameters such as pressures and saturations. All of the computer codes do this so the results can be evaluated and confirmed. While CCDFs are the basis for determining compliance, intermediate results are useful in reviewing the behavior of the system. For example plots such as those in Appendix SA and the PAVT (Docket A-93-02, Item II-G-28) uncertainty and sensitivity analysis (Docket A-93-02, Item II-G-30) show how pressure changes with time and the average volume of brine that is expected to be released.

The final results of the complete modeling process is collected into a set of CCDFs that are used to show results of the PA modeling for comparison with the §194.13 containment requirements. (CCA Chapter 6.5)

## 4.0 Important Modeling Issues

Performance assessment identifies what events could happen (scenarios), the likelihood that the events would occur, and estimates the cumulative releases of radionuclides from the potential events and processes. Scenarios are combinations of events and processes that may occur. They are developed from examining potential processes that occur if the site remains undisturbed by human intrusion (drilling) or if the site is disturbed or intruded. The disturbed scenario consists of all of those events and processes expected for the undisturbed case but with additional processes related to drilling, such as movement of waste from the repository to the surface through an intrusion borehole. In the undisturbed scenario a limited number of important processes are expected to occur, but none have enough impact singly or in combination to violate the individual and groundwater protection requirements. In addition existing features, such as the stratigraphy of the disposal system or rock matrix transport characteristics are important in modeling processes. DOE thus considers features, events and processes in the CCA PA calculations.

### 4.1 Computational Scenarios

In order to model the WIPP features, events and processes (FEPs), DOE constructed six scenarios in the CCA PA calculations, denoted S1 to S6 (Section 6.3, pp. 6-61 to 6-79 and the Validation Document for CCDFGF (Docket A-93-02, Item II-G-3, Volume 3, pp. 54-59). These six computational scenarios used in the CCA PA calculations are as follows:

- S1 - is the undisturbed scenario,
- S2 - is an E1 scenario where a borehole passes through the waste and into a Castile brine pocket at 350 years,
- S3 - is an E1 scenario where a borehole passes through the waste and into a Castile brine pocket at 1000 years,
- S4 - is an E2 scenario where a borehole passes through the waste and misses the Castile brine pocket at 350 years,
- S5 - is an E2 scenario where a borehole passes through the waste and misses the Castile brine pocket at 1000 years, and
- S6 - is an E2E1 scenario where two boreholes pass through the waste, one that misses the Castile brine pocket at 800 years and one that drills into a Castile brine pocket at 2000 years.

The first of these six scenarios is the undisturbed case; the other five are disturbed scenarios where human intrusion occurs. The time of intrusion calculated in scenarios S2 through S6 are selected to be located at times that gas generation impacts may be at their greatest. The

consequences of these scenarios are calculated by using a series of computer codes that implement the appropriate conceptual models.

The modeling of FEPs discussed here directly or indirectly relates to drilling into the repository and fluid injection. DOE proposed three major release mechanisms during a drilling intrusion: 1) Cuttings and Cavings, 2) Spallings, and 3) Direct brine release of radioactive materials; these are discussed further below. Long-term groundwater release through the Culebra dolomite and the Salado anhydrite markerbeds is a fourth possibility, but it has a negligible effect on releases even in the PAVT (see Figure 7.5 in Docket A-93-02, Item II-G-28). In addition the discussion will focus on FEPs that have the greatest influence on releases from the repository or which have been the source of public comment, including characteristics of the repository, waste reactions, actinide solubility, and retardation in the Culebra.

#### 4.2 Effect of Passive Institutional Controls on the Drilling Rate

Passive institutional controls (PICs) have been used by DOE as a method to potentially deter human intrusion (i.e., reduce the drilling rate) after credit for active institutional controls ends. The effectiveness of passive institutional controls has been questioned by EPA and public comments. This section briefly examines the probability of intrusions with and without PICs.

§194.33 directs DOE to identify the shallow and deep drilling rate over the past 100 years in the Delaware Basin and use that rate in modeling consequences over the 10,000 year regulatory time frame. DOE noted that shallow drilling (< 2150 feet or 655 meters) can be screened out from PA calculations based on low consequence. Deep drilling (> 2150 feet or 655 meters) was retained in the PA. The CCA indicates that there are essentially no releases unless there is a drilling intrusion into the repository. DOE identified that almost all of the deep drilling over the past 100 years can be attributed to oil and gas exploration and production. DOE calculated the rate of 46.8 boreholes per square kilometer per 10,000 years ( $\text{bh}/\text{km}^2/10^4$  years). The area in the repository occupied by contact- and remote-handled waste is 0.126 square kilometers. DOE assumed that the first 100 years have no drilling intrusions, years 100 to 700 have passive institutional controls that limit the drilling rate by two orders of magnitude below the drilling rate for a drilling rate of  $0.468 \text{ bh}/\text{km}^2/10^4$  years ( $0.01 * 46.8$ ), and the remaining 9300 years have the full drilling rate of  $46.8 \text{ bh}/\text{km}^2/10^4$  years.

Applying the drilling rate to the waste area after passive institutional controls are assumed to cease their effectiveness produces the probabilities of intrusions listed in Table 2 of this technical support document (assuming 0 to 100 years with no drilling due to active institutional controls, for 9300 years the drilling rate is assumed to be  $46.8 \text{ bh}/\text{km}^2/10^4$  years):

Table 2

Probability and Cumulative Probability of Number of Intrusion Boreholes for 9300 Years at WIPP

No of Boreholes	Probability	Cumulative Probability
0	0.004	0.004
1	0.023	0.027
2	0.062	0.089
3	0.114	0.203
4	0.156	0.359
5	0.172	0.531
6	0.157	0.688
7	0.123	0.811
8	0.084	0.895
9	0.051	0.946
10	0.028	0.974
11	0.014	0.988
12	0.006	0.994
13	0.003	0.997
14	0.001	0.998

Table 2 suggests that modeling intrusions after about the fourteenth intrusion is unnecessary because of the low probabilities at the drilling rate of 46.8 boreholes per square kilometer over 10,000 years.

As identified in Sandia National Laboratories impact analyses (WPO #41883 and WPO #41870) and EPA's sensitivity analysis (Docket A-93-02, Item V-B-13), DOE's plan to take a credit for passive institutional for 600 years does not have much of an effect on releases. DOE did not take credit for PICs in the PAVT because of Agency concerns about the effectiveness of PICs. The small effect of passive institutional controls is illustrated in a comparison of the following table with the previous table. The following table, Table 3, is calculated similarly to Table 2, except that no credit is assumed for passive institutional controls; therefore 9900 years is the time span used.

Table 3  
Probability and Cumulative Probability of Number of Intrusion Boreholes for  
9900 Years at WIPP

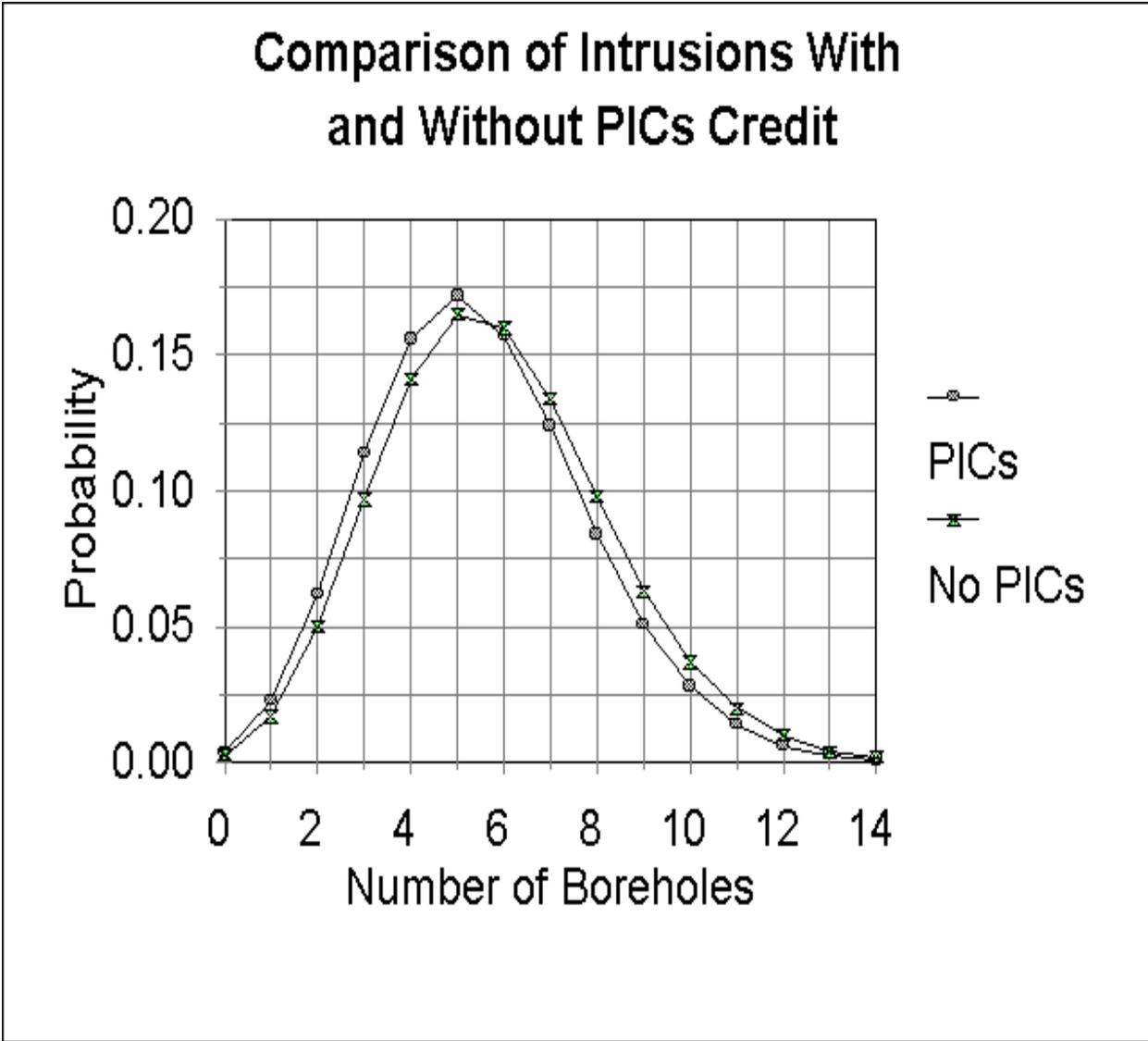
No of Boreholes	Probability	Cumulative Probability	Change in Probability For PICs and no PICs
0	0.003	0.003	0.001
1	0.017	0.02	0.006
2	0.05	0.07	0.012
3	0.097	0.167	0.017
4	0.141	0.307	0.015
5	0.165	0.472	0.007
6	0.160	0.632	-0.003
7	0.134	0.766	-0.009
8	0.098	0.864	-0.014
9	0.063	0.927	-0.012
10	0.037	0.964	-0.009
11	0.02	0.983	-0.006
12	0.01	0.993	-0.004
13	0.004	0.997	-0.001
14	0.002	0.999	-0.001

Figure 2 of this technical support document provides a graphic representation of the limited effect of passive institutional controls. In addition Figure 2 illustrates that, while limited, the credit for passive institutional controls is limited primarily to the borehole numbers 1 through 5. After the fifth borehole into the repository, there is essentially no credit for PICs.

The discussion so far has focused on multiple boreholes into the entire repository. However, the DOE conceptual model for WIPP assumes that two boreholes have to hit the same panel before there can be a multiple borehole scenario. Using the CCA drilling rate and applying the same CCA drilling rate of 46.8 bh/km<sup>2</sup>/10<sup>4</sup> years to one panel (assuming ten panels so the waste area is (0.126 km<sup>2</sup>)/10) produces the following:

Table 4  
Probability of Multiple Boreholes Into One Panel

No of Boreholes	Probability	Cumulative Probability
0	0.578	0.578
1	0.317	0.895
2	0.087	0.982
3	0.016	0.998
4	0.002	1.000



**Figure 2** Graphical representation of Table 3. Comparison of the probability of intrusions with credit for passive institutional controls (9300 years with a drilling rate of 46.8 bh/km<sup>2</sup>/10<sup>4</sup> years) and no credit allowed for passive institutional controls (9900 years with a drilling rate of 46.8 bh/km<sup>2</sup>/10<sup>4</sup> years).

Table 4 shows that the probability of multiple drilling hits into one panel is quite small, and it is very unlikely that more than three intrusions will occur into the same panel.

#### 4.3 Characteristics of the Repository

Characteristics and processes in the repository itself will affect potential releases, at least in a drilling intrusion. The Salado consists primarily of halite (salt) with some anhydrite (calcium sulfate) interbeds, and some clay seams. The halite will deform, creep, and crush the waste. The repository closure process will decrease porosity and increase pressure in the repository. The anhydrite interbeds may fracture and serve as a sink and pathway for gas generated in the repository if the pressure becomes high enough. If the anhydrite does fracture due to gas generation, gas pressure in the waste region would be reduced. Small volumes of brine are present in the Salado and small amounts may flow into the waste region at low rates. After closure of the repository in about 300 years, the potential amount of void volume is over 5,000 cubic meters per panel. The void volume will be occupied primarily by gas, unless fluid enters the repository through an intrusion borehole from a deeper Castile brine pocket or shallower water producing zone such as the Culebra Dolomite.

#### 4.4 Cuttings and Cavings

Drill bits in the Delaware Basin are typically 0.3115 meters (12.25 inches) in diameter. The radius is thus  $(0.3115 / 2) = 0.15575$  meters. The amount released from cuttings is simply the area ( $A = \pi r^2$ ) of the drillbit times the height of the removed material. The area of the drill bit is  $(0.15575 \text{ m})^2 * 3.14 = 0.076 \text{ m}^2$ . Therefore,  $0.302 \text{ m}^3$  ( $0.076 \text{ m}^2 * 3.96 \text{ m} = 0.302 \text{ m}^3$ ) is the volume of equivalent uncompacted waste which would be removed during a drilling intrusion. In the cuttings and cavings release, the material released is a function of the drill bit diameter and that which gets eroded from the borehole wall by the drilling fluid. The parameter TAUFAIL (resistance to erosion) controls the cavings--the lower TAUFAIL, the higher the cavings releases. In the CCA (and PAVT) the shear strength of the waste was the most important parameter to overall releases. DOE estimates in the CCA that an average waste volume of 0.3 - 3  $\text{m}^3$  would be removed by cuttings and cavings. CCA Appendix SA 3 states that "The release of more than 10 cubic meters of material is unlikely." EPA disagreed with DOE's method of arriving at the value for TAUFAIL and directed DOE (Docket A-93-02, Item II-I-27), in the PAVT, to base the value on the expert elicitation results (also see Technical Support Document for Section 194.23: Parameter Justification Report, Docket A-93-02, Item V-B-14 and CARD 26-Expert Judgment, Docket A-93-02, Item V-B-2). The range of the volume of cuttings and cavings was larger for the PAVT (range ~0.3 to 3.9  $\text{m}^3$ ) than for the CCA (range ~0.4 to 2.9  $\text{m}^3$ ) (Docket A-93-02, Item II-G-28).

## 4.5 Spallings

Spallings are the solid materials that are released if the repository gas pressure exceeds the hydrostatic pressure of the vertical column of the drilling fluid in the borehole. Spallings is one of the major release mechanisms in the CCA. DOE estimates that a waste volume of 0.5 - 4 m<sup>3</sup> would be removed from this mechanism when repository pressures are greater than about 8 megapascals (MPa). In the CCA particle diameter size is the major determinant of the volume of spallings material released. Particle sizes were estimated by DOE to be in the range of 40 microns to 20 centimeters ( $4 \times 10^{-5}$  m to 0.2 m) and releases were inversely related to particle size (Appendix SA 4). EPA reviewed the basis for DOE's estimate of the waste particle diameter used in the CCA and determined that it was not adequate and required an expert judgment panel to review the issue (A-93-02, II-I-27). DOE convened the expert panel with the result that the expert panel believed the particle size diameter would be larger than that used in the CCA (WPO #46936).

The Conceptual Model Peer Review Panel (CMPRP) found the spallings model implemented in the CCA to be inadequate, and so DOE conducted a significant computational and experimental program to develop a new spallings conceptual model. The new spallings modeling predicts extremely small spallings volumes for all gas pressures below lithostatic pressure. EPA has concluded that, since the spallings model in the CCA considers only particle dislodgement from the waste, not lofting of dislodged particles up the borehole, the approach taken by DOE is conservative. DOE assumes that all failed waste is transported to the surface when, in actuality, only a portion of the failed waste would be able to travel up the borehole, resulting in radioactive releases to the earth's surface. EPA does not believe that larger particles dislodged from the surfaces of radial fractures in the waste will be lifted 2150 ft to the land surface. The maximum size of particle which could be transported (assuming that adequate fluid energy was available) is limited by the annular space between the drill collar and the borehole wall. As discussed earlier, EPA agreed with the Conceptual Model Peer Review Panel that the spallings conceptual model was inadequate but the results were reasonable for use in PA (Docket A-93-02, Item II-G-22; Section 7 of the Technical Support Document for Section 194.23: Models and Codes, Docket A-93-02, Item V-B-6).

In the PAVT, DOE sampled the CCA predicted spallings releases (0.5 to 4.0 m<sup>3</sup>) when the repository pressure was greater than 8 megapascals (A-93-02, Items II-G-26 and II-G-28). This change in the modeling is captured in the new parameter VOLSPALL. When a spallings event occurred in the PAVT, the range for VOLSPALL was sampled using the CCA range of volumes released. In the CCA, the amount of spallings releases was determined by PARTDIA (CCA Appendix SA 3) when the pressure was greater than 8 megapascals.

## 4.6 Direct Brine Release

In the direct brine release scenario, pressure in the repository forces brine up the borehole, potentially to the Culebra and the surface. DOE estimates that a brine volume of 0 - 30 m<sup>3</sup> with dissolved waste, on average, would be removed from this mechanism. Assuming there is brine saturation in the repository, the amount of waste material brought up during a direct

brine release depends on the solubility and repository pressure. As stated in Appendix SA 6: “The direct brine release model predicts a release of brine (cubic meters). For a given drilling intrusion, the volume of released brine is multiplied by the concentration (EPA units per cubic meter) of dissolved radionuclides in contact-handled transuranic (CH-TRU) waste (Section SA.7) at the time of the intrusion to produce the direct brine release. Prior to an E1 intrusion, solubilities associated with brines derived from the Salado are used; after an E1 intrusion, solubilities associated with brines derived from the Castile are used.” Remote handled transuranic (RH-TRU) waste does not contribute to direct brine release (Appendix SA 6). Since RH-TRU waste is emplaced in the halite walls of the repository, the low permeability of the halite is expected to prevent the RH-TRU waste from getting dissolved and transported with the CH-TRU waste. The largest volume of direct brine released in the CCA is 55 m<sup>3</sup>. In the PAVT the largest brine volumes released were, for each replicate, respectively, 108 m<sup>3</sup>, 1,200 m<sup>3</sup>, and 105 m<sup>3</sup> (Docket A-93-02, Item II-G-28).

#### 4.7 Waste Reactions

While the waste inventory consists of many components, those components of most interest are the metals and biodegradable materials (cellulosics and potentially plastics). Metals will corrode, producing gas. Microbial respiration, of biodegradable materials could also produce gas for up to about 1000 to 2000 years (see, for example, Figure A.1-7 in Docket A-93-02, Item II-G-26). In the conceptual model for gas generation, DOE identified that the presence of future microbes at the WIPP is unknown and assumed that 50% of the time microbes would not be viable (Appendix PEER 3.21.2.2). In the 50% of the time that microbes were assumed to survive, the microbes were assumed to degrade cellulosics only or cellulosics, plastics and rubber.

The resulting pressure from gas production is important in determining how much material gets released in spallings and direct brine release events. Brine is necessary to corrode the metals as well as provide a suitable environment for microbial activity to generate gas. Magnesium oxide (MgO) is planned as a backfill, the primary purpose of which is to stabilize or decrease the solubility of actinides in the brine by buffering potential repository fluids around a pH of 9. An important secondary effect is to react with CO<sub>2</sub> (produced from microbial degradation of waste) in the gas phase. This reaction is expected to reduce the CO<sub>2</sub> partial pressure, and hence the overall pressure in the repository. Other supplemental effects of the MgO is to cement the waste as MgO reacts with water, and the removal of water from the waste decreasing its water saturation.

#### 4.8 Actinide Solubility

In a direct brine release scenario, actinides that are dissolved in brine may move up the borehole if there is enough pressure and brine in the repository. With the addition of magnesium oxide DOE believes the range of median actinide solubilities can be narrowed to between 10<sup>-6</sup> and 10<sup>-9</sup> moles/liter (see Table 5 in this technical support document for the median actinide solubility values used in the CCA and PAVT).

A conceptualization of the redox environment within the repository is important to predicting the solubilities of probable solids incorporating actinide species. Actinides can exist in oxidation states ranging from +3 to +6, depending on the specific actinide under consideration and prevailing redox conditions. After closure, the repository is expected to become anoxic relatively rapidly because of reactions between any available oxygen and iron metal and aerobic biodegradation of organic material (CCA Appendix SOTERM 2.2.3). Both organic materials and iron metal are expected to be major components of the waste inventory. According to DOE (CCA Appendix SOTERM 4.6) “each drum contains about 170 moles of iron in the container... The reaction rate of iron with the brine is very fast (Appendix PAR, Parameter 1). Therefore, as any brine moves into the repository it will react with the iron and establish a highly reducing environment.” Additionally, the production of hydrogen by metal corrosion reactions is expected to contribute to creating reducing conditions in the repository. The assumption of reducing conditions after closure is reasonable because of the interaction of the iron and brine. Because of these reactions, oxidizing conditions are expected to last only a short while after closure. EPA therefore concurs with DOE that reducing conditions will prevail in the repository after closure.

DOE presents the experimental and chemical bases for the determination of the specific oxidation states for each actinide expected to be predominant in the repository (Appendix SOTERM 4; CCA Reference 479). Actinide chemistry indicates that specific oxidation states can be expected under reducing conditions (CCA Chapter 6.4.3.5; Appendix SOTERM 4). Americium is expected to be present in primarily the +3 oxidation state. Higher oxidation of Am(+5) and Am(+6) can occur under oxidizing conditions, but are rapidly reduced by naturally occurring reductants and in brines at pH greater than 9 (CCA Reference 247). Plutonium is expected to be present as either Pu(+3) or Pu(+4). Pu(+5) and Pu(+6) are not expected to be dominant oxidation states for Pu under the reducing conditions of the repository and abundance of metallic iron. Uranium is expected to exist in both the +4 and +6 oxidation states; the predominance of which could not be ascertained based on current knowledge or uranium chemistry. The predominance of U(+4) requires extremely reducing conditions, that while possible for the repository, cannot be predicted with certainty. Consequently, for the PA, uranium is designated as being present as U(+4) in 50% of the runs and as U(+6) in the other 50%. Uranium is present in very low quantities in the repository and is not discussed further in this summary, except in reference to the comparison of the CCA to the EPA-Mandated PAVT discussed in Section 5.

DOE assumed that with the addition of MgO, magnesite would be the stable magnesium form. However, magnesite may not be the stable magnesium mineral. EPA believes that hydromagnesite will be the long-term metastable mineral phase. EPA’s analysis of the solubility calculations using the Fracture-Matrix Transport (FMT) code indicated that DOE did not take into account the possibility of hydromagnesite as a metastable mineral species in the stability reaction, which would impact the calculated solubility values. EPA identified that the database used for FMT was in error; DOE subsequently changed it to account for the presence of hydromagnesite. EPA re-ran the actinide solubility analyses (refer to EPA’s Technical Support Document for Section 194.24: EPA’s Evaluation of DOE’s Actinide Source Term, Docket A-93-

02, Item V-B-17). EPA's results indicate that modified solubility values for actinides are required, and EPA-Mandated PAVT was run using these values. Table 5 lists the actinide solubilities used in the CCA and the PAVT. DOE has since performed experiments which identify hydromagnesite as a metastable mineral species (Docket A-93-02, Item II-A-39). With hydromagnesite as the expected magnesium mineral species, the actinide solubility is expected to be lower than that used for the CCA.

DOE defined uncertainty limits for actinide concentrations calculated from solubility relationships based on the differences between measured concentrations and those predicted for the solubilities of discrete actinide solids with the FMT or NONLIN computer codes (WPO #41374). These differences were measured for a number of experimental studies of the solubilities of different actinide solids in high ionic strength solutions. Bynum (WPO #41374) used data only from solubility experiments with +3 and +5 actinides to construct the uncertainty distributions because of experimental data quality. These uncertainty limits were determined by DOE to range from 1.4 log units above to 2.0 log units below the actinide concentrations calculated from solubility expressions contained in the FMT model. These uncertainty parameters were used for each actinide sampled in the PA, that is for Am(III), Pu(III), Pu(IV), in Castile and Salado brines, U(IV) in Salado brine, U(VI) in both Castile and Salado brine, and Th(IV) in Salado brine. Table 6 of this technical support document lists the CCA median actinide solubilities and high end of the solubility range after the uncertainty range is applied.

Table 5

PAVT and CCA Solubilities (moles/liter) of Actinide Oxidation States in Salado and Castile Brines Controlled by the MgO/MgCO<sub>3</sub> Buffer

Brine Source	+ III		+ IV		+ V		+ VI	
	PAVT	CCA	PAVT	CCA	PAVT	CCA	PAVT	CCA
Salado	1.2 E-7	5.8 E-7	1.3 E-8	4.4 E-6	2.4 E-7	2.3 E-6	8.7 E-6	
Castile	1.3 E-8	6.5 E-8	4.1 E-8	6.0 E-9	4.8 e-7	2.2 E-6	8.8 E-6	

Table 6  
CCA Actinide Solubilities and the Upper Limit (moles/liter)

Brine Source	+ III		+ IV		+ V		+ VI	
	CCA	CCA * 10 <sup>1.4</sup>						
Salado	5.8 E-7	1.46 E-5	4.4 E-6	1.1 E-4	2.3 E-6	5.78 E-5	8.7 E-6	2.19 E-4
Castile	6.5 E-8	1.63 E-6	6.0 E-9	1.51 E-7	2.2 E-6	5.53 E-5	8.8 E-6	2.21 E-4

#### 4.9 Releases in the Salado Anhydrite Markerbeds and in the Culebra Dolomite

While direct releases to the surface are probably the most important pathway for radionuclide release, the Salado anhydrite markerbeds and the Culebra Dolomite, approximately 300 meters above the repository, have also been considered as potential pathways for radionuclide release. As mentioned earlier, the Salado anhydrite markerbeds have a low permeability, only slightly higher than the salt. The markerbed permeability can increase if it is fractured, but fracturing is not a significant problem in the undisturbed case. The anhydrites are not a major pathway to the accessible environment during intrusion events; the borehole replaces the anhydrites as the preferred pathway in the disturbed case. Only nine realizations in the CCA undisturbed calculations had radionuclide transport to the accessible environment through the anhydrites, and--because the releases were so low--these realizations may have been a result of numerical dispersion in the computer code calculations instead of actual releases. Releases through the anhydrites in the Salado therefore are not a source of significant releases.

Due to the extremely low permeability of the Salado halite blocking radionuclide migration from the waste, it is necessary to have an intrusion to provide a pathway from the waste to the Culebra. The physical character of the Culebra with respect to groundwater transport is conceptualized as having dual-porosity(e.g. flow occurs in both rock fracture and rock matrix). The medium is conceptualized as consisting of 1) advective porosity, where solutes are carried by groundwater flow in fractures, and as 2) fracture-bounded zones of diffusive porosity, where solutes move through rock matrix via slow advection or diffusion (SAND97-0194). The advective porosity incorporates interconnected fractures and vugs and irregular interbeds of silty dolomite. The diffusive porosity predominately represents the porosity of the dolomite matrix. Actinide transport is retarded both physically and chemically when diffusion out of the advective porosity and into the dolomite matrix occurs. Physical retardation occurs because actinides that diffuse into the matrix are essentially removed from transport by groundwater flow, at least until the actinides diffuse back into the advective porosity. Chemical retardation occurs within the rock matrix as a result of adsorption of actinides onto the dolomite. The relationship between the sorbed and liquid concentrations of actinide is represented by  $K_d$ s. In the transport computer codes, the distinction between advective and

diffusive porosity is important because partitioning of actinide to the dolomite is considered only for the groundwater migrating through diffusive porosity zones.

The 1992 PA (CCA reference 563, Chapter 8) indicated that if radionuclides managed to get to the Culebra, and no retardation of the actinides occurred, then the actinides could get to the WIPP boundary rather quickly. The 1996 CCA takes credit for radionuclide retardation in the Culebra, and as a result, radionuclides appear to travel less than several hundred meters in any quantity; most of the radionuclides migrate less than 50 meters. DOE's modeling of groundwater flow and transport in the Culebra indicates that even low (1- 3 ml/g; Marietta and Larson, 1997, WPO #47414) chemical retardation values ( $K_d$ s)--lower than those used in the CCA--are enough to stop the transport of radioactive materials to the Land Withdrawal Boundary. In addition, continued experimental work reinforces DOE's selection of  $K_d$  values. As of July, 1997 (post-CCA), breakthrough was not observed for Pu, Am, and Th (letter from G. Dials to R. Neill, Attachment 2, Docket A-93-02, Item II-D-115). Minimum  $K_d$ s of at least 100 ml/g were calculated for these strongly retarded actinides. Destructive analysis of one core indicated that most of the Am and Pu remained within the top few millimeters of the core (Perkins, 1997, WPO #47414).

Modeling was performed by EPA to evaluate the effect of  $K_d$  on transport of radionuclides in the Culebra. Low-end  $K_d$  values from the CCA were simulated for U ( $3.0 \times 10^{-5}$  m<sup>3</sup>/kg) and Am and Pu ( $0.02$  m<sup>3</sup>/kg) using the transport code STAFF3D and the mean transmissivity field from the 1992 PA (Docket A-93-02, Item V-B-6, Section 12, and Docket A-93-02, Item V-B-7). Assuming a network of 10 fractures, breakthrough occurs at the downgradient edge of the land withdrawal boundary at about 3,000 years for uranium. Breakthrough does not occur at relative concentrations greater than  $1 \times 10^{-5}$  during the 10,000 year simulation for Am or Pu. For a scenario in which 100 fractures are simulated, no breakthrough is observed at relative concentrations greater than  $1 \times 10^{-5}$  during the 10,000 year simulation for U, Am or Pu. The results of these model simulations are in reasonable agreement with the results of the CCA and the PAVT.

#### 4.10 Fluid Injection

DOE stated that oil and gas extraction includes fluid injection activities, primarily waterflooding and brine disposal. Stoelzel and O'Brien (CCA, reference #611) evaluated the effects of fluid injection from two hypothetical boreholes near the WIPP using the BRAGFLO code, with some modified parameters and assumptions to fit the fluid injection conditions (e.g., a modified grid system). Stoelzel and O'Brien's report concludes that although a worst case realization did result in brine inflow from the injection location to the repository over an approximately two-mile distance within anhydrite interbeds of the Salado, the volume of cumulative brine inflow was relatively small and within the bounds of brine inflow values calculated for the undisturbed scenario of the CCA PA. Therefore, DOE eliminated the fluid injection FEP based upon low consequence.

The CCA and supplementary information on fluid injection show that there is little consequence of fluid injection activities. The supplemental information provided by DOE

indicates that current well construction methods makes it unlikely that there could be a well failure of the nature that occurred in the Rhodes-Yates field outside the Delaware Basin (Docket A-93-02, Item II-I-36, section b.1). DOE's analysis used reasonable estimates and concepts to screen out the fluid injection scenario as inconsequential. Although DOE did not use probability of failure to rule out fluid injection, DOE's analysis of well construction and operating practices around WIPP also shows that there is a very low probability that a well would suffer a complete failure.

DOE identified the Bell Canyon Formation under the Salado and Castile Formations as the primary target for fluid injection for brine disposal. DOE modeled the fluid injection scenario using WIPP geology, and again using the geology identified in the Rhodes-Yates Field. The two sites differ significantly because the Castile Formation, which underlies the Salado at the WIPP, is absent in the Rhodes-Yates Field. DOE assumed that fluid injection activities would occur continuously for 50 years, and evaluated the subsequent effects of such injection activities over the entire 10,000-year regulatory time frame. The modeling results indicated that some brine could potentially get into the WIPP from fluid injection activities. However, the amount of brine from the worst case scenario (the "Rhodes-Yates" scenario) was low compared to the amount of brine expected to enter the waste area naturally. DOE thus screened out the fluid injection scenario on the basis of low consequence.

EPA's review of the CCA raised additional questions regarding DOE's screening analysis of fluid injection. EPA believes that 50 years is an accurate estimate for the life of a single oil field, but that it does not account for the possibility of multiple fields. Because drilling restrictions currently applicable to potash areas in the Delaware Basin could be lifted, it is possible that multiple oil fields could be developed in the foreseeable future near the WIPP. Based on the current resources and leases in the vicinity of the WIPP, EPA estimated that oil could still be drilled up to 150 years from now. EPA thus required DOE to extend the 50-year time frame in its models to 150 years. EPA also required DOE to use modified values for some input parameters, and to model the behavior of the disturbed rock zone consistent with assumptions used in the PA. (Docket A-93-02, Item II-I-17) Finally, EPA required DOE to provide additional information on the frequency of fluid injection well failures.

In supplemental work on fluid injection, DOE addressed all the issues identified by EPA. DOE modified the computer model grid configuration and added a new model to address concerns raised by both EPA and stakeholders. DOE researched injection well operating practices and construction in the Delaware Basin and identified significant differences between those in the vicinity of the WIPP and the Rhodes-Yates Field. For example, wells near the WIPP are typically less than ten years old and are constructed to much higher mechanical standards than the older, less robust wells found in the Rhodes-Yates Field. DOE identified a range of well failure scenarios, from undetectable brine flow to catastrophic well failure. DOE's data indicated that the probability of a catastrophic well failure in the vicinity of the WIPP is extremely low. DOE confirmed that the presence of the Castile at the WIPP also substantially inhibits injected brine movement into the Salado anhydrite markerbeds.

Public comments on this issue included a detailed report that contradicted the DOE fluid injection modeling and indicated that fluid injection activities could overwhelm the WIPP with brine. (Docket A-93-02, Item II-H-28) EPA has reviewed the report and considers it to model conditions that are highly unrealistic for the WIPP. For example, all modeled scenarios assumed that the entire volume of brine was injected directly into the anhydrite marker beds in the Salado Formation. In addition, the report (Docket A-93-02, Item II-H-28) modeled the occurrence of fluid injection well beyond the time frame contemplated by §194.32(c). The report also ignored current well construction and fluid injection operating practices, which are more robust than that used in the 45-year-old Rhodes-Yates Field.

EPA agreed with commenters that the original fluid injection screening was not adequate. Thus EPA required DOE to provide additional information and to do additional modeling. The additional modeling showed rates of brine inflow (and thus effects on the disposal system) even smaller than those estimated by the original CCA screening analysis. DOE provided documented evidence that the well construction and operating practices near the WIPP are much more robust than that in the Rhodes-Yates well. Both DOE's research and EPA's own review of fluid injection (Technical Support Document for Section 194.32: Fluid Injection Analysis, Docket A-93-02, Item V-B-22), indicated that the probability of a long-term fluid injection well failure is below the regulatory cutoff of 1 in 10,000 over 10,000 years. Based on DOE's modeling and examination of fluid injection practices, EPA believes that a salt water blowout situation in the Rhodes-Yates Field is extremely unlikely to occur and affect WIPP's ability to contain radionuclides. Thus, EPA concurs with DOE that fluid injection is a low-probability scenario that can be screened out of the PA based on low consequence.

#### 4.11 Anhydrite Markerbeds

The Salado markerbeds' response to pressure increases from fluids (gas and brine) is important to understanding the performance of the WIPP. Gas generation, discussed earlier, is a process that acts on the anhydrites from within the waste region. In the fluid injection scenario, brine is injected into the anhydrites from outside the controlled area.

Salado markerbeds contain natural fractures that may be partially healed. If high pressure is developed in an interbed, either from gas generation or brine flow from within the repository or from brine injection from outside the repository, its preexisting fractures may dilate or new fractures may form, altering its porosity and permeability. Pressure-dependent changes in permeability are supported by experiments conducted in the WIPP underground and in the laboratory (Beauheim et al. 1993, WPO 23378). Accordingly, DOE has implemented in BRAGFLO a porous-media model of interbed dilation and fracturing that causes the porosity and permeability of a computational cell in an interbed to increase as its pore pressure rises above a threshold value. To the extent that it occurs, dilation or fracturing of interbeds is expected to increase the transmissivity of interbed intervals. The threshold pressure of dilated or fractured interbeds is expected to be low because apertures of the fractures increase; thus, fluid is expected to be able to flow outward readily if adequate pressure is available to dilate the interbeds.

The model used in BRAGFLO to simulate the effects of interbed dilation or fracturing assigns a fracture initiation pressure above the initial pressure at which local fracturing takes place, and changes in permeability and porosity occur above this pressure (Appendix BRAGFLO 4.10). Interbeds have a fracture-initiation pressure above which local fracturing and changes in porosity and permeability occur in response to changes in pore pressure. A power function relates the permeability increase to the porosity increase. A pressure is specified above which porosity and permeability do not change.

Below this fracture initiation pressure, an interbed has the permeability and compressibility of intact rock as assigned by Latin Hypercube Sampling (see Appendix A of the Technical Support Document for Section 194.23: Models and Computer Codes, Docket A-93-02, Item V-B-6). Below the fracture initiation pressure, the initial sampled porosity is modified slightly with pressure caused by compressibility. Above the fracture initiation pressure, the local compressibility of the interbed is assumed to increase linearly with pressure. This greatly alters the rate at which porosity increases with increasing pore pressure. Additionally, permeability increases by a power function of the ratio of altered porosity to initial porosity. For numerical reasons (that is, to prevent unbounded changes in parameter values that would create numerical instabilities in codes), a pressure is specified above which porosity and permeability change no further.

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

The purpose of this model is to alter the porosity and permeability of the anhydrite interbeds if their pressure approaches lithostatic, simulating some of the hydraulic effects of fractures with the intent that unrealistically high pressures (much in excess of lithostatic) do not occur in the repository or disposal system. The porosity and permeability increases are conceptualized as occurring vertically throughout the affected interbed; in other words, throughout the porous medium as a whole rather than on discrete portions. This simplification facilitates numerical implementation and execution.

The BRAGFLO fracture enhancement model assumes the propagation of fractures occur uniformly in the direction lateral to flow within the marker beds (Docket A-93-02, Item II-G-8, Section 3.6). The maximum enhanced fracture porosity controls the amount of storage within the fracture. The extent of the migration of the gas front into the marker bed is sensitive to this storage. The additional storage due to porosity enhancement will mitigate the fluid migration distance within the marker bed. The enhancement of permeability due to marker bed fracturing will make fluids more mobile and will contribute to longer migration distances. Thus the dual effects of porosity and permeability enhancement are tradeoffs in effecting migration distances.

The conceptual model for the fracturing of the anhydrite marker beds was judged to be adequate by the Conceptual Models Peer Review Panel. However, EPA raised several significant concerns regarding the uncertainty associated with the conceptual model and the

means by which it was implemented in the CCA (Docket A-93-02, Item II-I-17). Specifically, EPA believed that DOE had not provided an adequate defense for ruling out alternative mechanisms for fracture propagation, since there are several different hypotheses for how the fracturing could actually occur (Docket A-93-02, Item II-G-I, Volume XII, Appendix PEER, PEER-2). EPA was also not convinced that DOE had supported their contention that the fracturing model was based on data and not expert judgement, and that DOE had adequately treated the model uncertainties in the CCA.

To address these concerns, DOE provided additional information that explained the theoretical basis for the anhydrite fracture model and how the theoretical basis is supported by laboratory data (Docket A-93-02, Item II-I-24), and although there is still considerable uncertainty regarding the constitutive relationships of the fractures (i.e., relative permeabilities and capillary pressures), the fracture properties are based on laboratory and field data as described in (Larson et. al and Beauheim et al., 1994 referenced in Docket A-93-02, Item II-I-03; Beauheim et. al, 1993, WPO #23378). Furthermore, EPA believes that the uncertainty with respect to these parameters will be captured by the method in which DOE statistically samples the initial pressures at which fracturing is initiated. After reviewing DOE's documentation, EPA is satisfied that the Salado Interbeds Conceptual Model adequately represents the behavior of the system.

Bredehoeft and Gerstle (A-93-02, Items II-D-116 and II-D-118) have suggested that the linear elastic fracture mechanics model is more appropriate to WIPP than the DOE BRAGFLO porosity model. The alternative fracture model proposed by Bredehoeft and Gerstle is based on linear elastic fracture mechanics (LEFM). This model is based on the assumption that the anhydrite interbeds are a previously non-fractured, non-porous, homogeneous elastic medium. The report identifies gelatin as an example of such a medium. The reports correctly point out that fractures tend to occur as single features that can be very long in homogeneous elastic media, such as the gelatin described in the report. The reports state that the LEFM model does not predict the simultaneous generation of multiple fractures, even though such fractures were observed in DOE's field tests (Docket A-93-02, II-G-1, CCA Ref. #52) (see responses to comments for Anhydrite Fracturing, Response to Comments, Section 5).

The DOE's fracture model is based in part on the results of field tests at WIPP and in part on theoretical considerations (see A-93-02, V-B-14 and II-I-24). It recognizes that the anhydrite interbeds are previously fractured, bedded media containing open pores and voids through which brine can migrate. The open pore volume allows gas to enter at multiple locations and displace the resident brine when gas pressure is sufficiently high. Preexisting surfaces of weakness in the anhydrite result from natural fracturing and bedding planes and strongly influence the nature and occurrence of hydraulic fracturing. Field tests have created multiple planes of fracture propagation within the interbeds close to the point of injection.

The lack of similarity between the ideal homogeneous elastic medium upon which LEFM theory is based and the highly discontinuous, fractured anhydrite that forms the interbeds at WIPP is striking. Although EPA recognizes that accurate prediction of fracture propagation in natural rock is difficult, the DOE's fracture model incorporates actual field data, is based on a

more accurate representation of the anhydrite than the LEFM model, and is considered by EPA to provide a better predictive capability when compared to field data. EPA has thoroughly reviewed the DOE's porosity fracture model in BRAGFLO and the alternative Linear Elastic Fracture Mechanics (LEFM) model proposed by the commenter in the report referenced in the comment. The Agency has concluded that the model incorporated into BRAGFLO is expected to have a better predictive capability for the anhydrite interbeds at WIPP than the LEFM model.

#### 4.12 Actinide Inventory

The containment requirements for the WIPP at Section 191.13 are expressed in terms of normalized release. Normalized releases, in turn, are computed from estimates of radionuclide releases (in terms of activity in curies), the estimated waste unit factor (based on transuranic components of the total WIPP inventory), and the tabulated values of the release limits from Appendix A of 40 CFR Part 191. Very few of the radionuclides make up the bulk of the repository and dominate the release calculations.

Based upon waste emplacement and decay information, DOE concluded that the waste unit factor would be 4.07 (4.07 million curies of transuranic radionuclides) if disposal ceased in 1995 based on existing inventory projections (Appendix WCA, Table WCA-5, p. WCA-21). DOE obtained a waste unit factor of 3.44 at the time of disposal, year 2033, accounting for the decay of radioactive waste.

DOE used the waste unit factor of 3.44 to prepare sample calculations, to determine the release limits for radionuclides, to express the WIPP inventory and projected releases in "EPA units," and to present the relative contribution of each radionuclide to a normalized release. Of the 47 contributing radionuclides in the inventory, plutonium and americium isotopes were present in greatest abundance and consist of over 99% of the inventory at disposal. The top five radionuclides contribute to greater than 99.9 percent of the unit of waste value and to 99.4 percent of the initial EPA Units for CH-TRU and RH-TRU waste. The dominant CH-TRU radionuclides are:  $^{241}\text{Am}$ ,  $^{238}\text{Pu}$ ,  $^{239}\text{Pu}$ , and  $^{240}\text{Pu}$ . Table 7 of this technical support document lists the estimated inventory of these four radionuclides at discrete intervals for the 10,000 year period. After about year 3,000 the repository is almost entirely  $^{240}\text{Pu}$  and  $^{239}\text{Pu}$ . The two parent radionuclides  $^{241}\text{Pu}$  and  $^{244}\text{Cm}$  that produce  $^{241}\text{Am}$  and  $^{240}\text{Pu}$ , respectively, are also used in the calculations ( $^{238}\text{Pu}$  is also a parent to  $^{234}\text{U}$ ). For RH-TRU, there are three additional key radionuclides:  $^{137}\text{Cs}$ ,  $^{90}\text{Sr}$ , and  $^{233}\text{U}$ .

EPA reviewed DOE's calculation of the 2033 inventory, given the information in Appendices WCA and WCL. EPA found an error in DOE's calculation of the waste unit factor, but determined that the error was both small (5 percent impact on the computation of normalized releases) and in the direction that indicated more effective confinement of waste by the WIPP than had been thought previously.

Table 7

The CCA inventory for <sup>238</sup>Pu, <sup>239</sup>Pu, <sup>241</sup>Am, <sup>240</sup>Pu was decayed for 10,000 years in order to estimate the inventory over the regulatory time frame. These radionuclides were used because they constitute about 99% of the inventory after the 100 year period that active institutional controls are assumed to cease effectiveness. This information is used to estimate the curie concentration, for which a weighted average is derived in Table 8. With its short half-life, <sup>238</sup>Pu has decayed by about year 1000. <sup>241</sup>Am is nearly gone at 3000 years after closure. The plutonium 239 and 240 isotopes account for nearly all of the activity after 3000 years.

Actinide	<sup>238</sup> Pu	<sup>239</sup> Pu	<sup>241</sup> Am	<sup>240</sup> Pu		
Half-life, years	87.7	24,100	432	6,540		
Year from 2033	Curies	Curies	Curies	Curies	EPA Units per m <sup>3</sup>	Curies/m <sup>3</sup> using 176,000 m <sup>3</sup>
0	1,932,883	794,132	490,147	214,136	0.063*	19.5
100	876,912	791,851	430,491	211,878	0.038	13.1
500	37,150	782,794	219,742	203,084	0.021	7.1
1000	714	771,617	98,514	192,602	0.018	6.0
1500	14	760,600	44,166	182,661	0.016	5.6
2000	0	749,740	19,800	173,233	0.016	5.4
2500	0	739,036	8,877	164,292	0.015	5.2
3000	0	728,484	3,980	155,813	0.015	5.0
4000	0	707,830	800	140,144	0.014	4.8
5000	0	687,762	161	126,050	0.013	4.6
6000	0	668,263	32	113,374	0.013	4.4
7000	0	649,317	6	101,973	0.012	4.3
8000	0	630,908	1	91,719	0.012	4.1
9000	0	613,020	0	82,495	0.011	4.0
10,000	0	595,640	0	74,199	0.011	3.8

\*<sup>241</sup>Pu (half-life = 14.39 years) used in calculation at year 2033. The inventory contribution of <sup>241</sup>Pu at 100 years (~3,000 curies) and beyond is insignificant to the EPA unit calculation.

Table 8

Table 8 was created using the actinide concentration calculated in Table 7. After about 3000 years the curie activity is predominately from the plutonium isotopes <sup>238</sup>Pu and <sup>239</sup>Pu. This table and Table 7 can be used for comparisons to the solubility of the actinides. Depending on the time of interest, a particular radionuclide in solution may be solubility limited or inventory limited.

10,000 Year Weighted Average Actinide Concentration

Period (Years)	Average (Curies/m <sup>3</sup> ) per Period	Weighted Average (Curies/m <sup>3</sup> ) per Period	EPA Units per m <sup>3</sup> per Period	Weighted Average EPA Units per m <sup>3</sup> per Period
100 to 1,000	8.75	0.79	0.0254	0.0023
1,000 to 3,000	5.45	1.09	0.0158	0.0032
3,000 to 10,000	4.38	3.07	0.0027	0.0038
10,000 year Weighted Average =		<b>4.9 Curies/m<sup>3</sup></b>		0.0093 EPA Units per m <sup>3</sup>

## 5.0 EPA Mandated Performance Assessment Verification Test (PAVT)

EPA identified concerns with some parameter values (~1.5% of DOE's parameters) and computer codes. The PAVT was a set of 300 additional PA realizations (calculations) that tested the cumulative sensitivity of the parameter value changes identified by EPA. In addition, the PAVT addressed whether software problems identified by DOE would affect the results of the calculations. EPA's goal with the additional calculations of the PAVT was to verify that the cumulative impact of the changes to computer codes and parameters did not violate the radioactive waste disposal standards. That the results of the PAVT were well below the containment requirements of §191.13 and close to the original CCA results indicate that EPA directed changes to the parameter values and the changes DOE made to the computer codes were not significant enough to necessitate a new PA. The PAVT results thus verify that the CCA calculations are acceptable as the bases for EPA's compliance determination decision.

EPA directed DOE to demonstrate the combined effect of the parameter and code changes by conducting additional calculations in a PAVT. (Letters From Ramona Trovato to George Dials, April 17, 1997 and April 25, 1997, Docket A-93-02, Items II-I-25 and II-I-27.) The PAVT was an independent computer simulation of the WIPP's performance conducted under EPA's authority to require independent verification computer simulations (see §194.23(d)). The PAVT implemented DOE's PA modeling, using the same sampling methods as the CCA PA, but incorporating parameter values mandated by EPA. The methods used to execute the PAVT were identical, from a technical standpoint, to those used for the CCA PA. That is, DOE used the same computer codes, same sampling methodologies, etc., but changed the parameters identified by EPA and modified some of the computer codes in response to EPA's questions about the codes. The results included 300 CCDF curves, and were used to verify that the combined effect of computer code changes and altered parameter values do not significantly alter the results of the PA and certainly do not cause the predicted releases from the WIPP to violate the containment requirements.

The major changes to the software involved the SECOTP2D Culebra radioactivity transport code and the NUTS Salado radioactivity transport code. As part of the software change process, DOE/SNL conducted separate impact analysis of the software coding changes and identified that the impacts of the changes to the computer codes were small. The impacts of the changes were not great because in the Culebra little radioactivity reached the Culebra and the chemical retardation was modeled accurately enough in both the PAVT and CCA to identify that there were few or no releases to the accessible environment through the Culebra. The changes in NUTS were not significant either because the major error in the code involved using in the CCA the wrong, but higher, solubilities for several of the actinides.

### 5.1 Comparison of the PAVT and CCA Results

Table 9 of this technical support document lists the individual releases identified from the graphs in the supplementary PAVT report (Docket A-93-02, Item II-G-28). Figure 1 from the same report portrays the summary CCDFs for both the CCA and PAVT. The following are some observations that can be drawn from Table 9.

- The changes to the parameters in the PAVT produced higher releases than those presented in the CCA.
- In the CCA and PAVT, cuttings/cavings and spillings release processes [produce similar releases], however, the PAVT results are about two to three times greater than the CCA for most releases. The difference is greatest for direct brine releases at the 0.001 probability and least for the spillings at the 0.001 probability.
- In the CCA, short-term direct brine releases (directly to the surface) are very small at the probabilities of 0.1 and 0.001. At the 0.001 probability for both the CCA and PAVT, direct brine releases do contribute to total releases, and more for the PAVT. EPA's review identified that the CCA PA had potentially overestimated solubilities by about a factor of 10 in some cases, and thus lowered the solubilities for the PAVT (except for U(VI) which stayed the same). As a result, the direct brine releases are lower in the PAVT than they would have been if the CCA solubilities had been used.
- Culebra (long-term brine) releases are insignificant in both the PAVT and CCA for all probabilities, although the PAVT releases were non-zero at the 0.001 probability. This was due to the increased number of realizations in which uranium reached the accessible environment in the PAVT compared to the CCA (Docket A-93-02, Item II-G-30).
- In both the CCA and PAVT at the 0.1 probabilities, neither mean curve was greater than 0.2 EPA units versus the 1 EPA unit of the regulation. Neither the CCA or the PAVT mean curve was greater than 1 at the 0.001 probability (compare this to the disposal standard of 10 EPA units at the 0.0001 probability).

## 5.2 Specific PAVT Issues

- Changes in parameter values or ranges of parameter values at EPA's direction included actinide solubilities (6 parameters), brine pocket characteristics (2 parameters), intrusion borehole plug permeability (short- and long-term), chemical retardation or  $K_d$ s (6 parameters), shear resistance parameter that controls the amount of cavings expected (1 parameter) and the corrosion rate (1 parameter). Other parameters changed were the waste permeability, disturbed rock zone permeability, the angular drill bit velocity. The complete list of parameters changed for the PAVT is listed in Table 10 of this technical support document. Table 11 list the parameters that had the greatest effect on releases in the CCA and the PAVT. The Technical Support Document for Section 194.23: Parameter Justification Report (Docket A-93-02, Item V-B-14) provides the rationale for EPA's selection of the parameter values used in the PAVT.
- The average range of the volume of cuttings and cavings was larger for the PAVT (range ~0.3 to 3.9 m<sup>3</sup>) than for the CCA (range ~0.4 to 2.9 m<sup>3</sup>) (Docket A-93-02, Item II-G-28).
- In the CCA and PAVT the shear strength of the waste (TAUFAIL) was the most important parameter to affect overall releases. Table 11 of this technical support document lists the

most important parameters for individual release mechanisms for the PAVT and CCA. Table 12 lists the results from the DOE stepwise regression analysis. Table 12 indicates the relative importance of the parameters on releases.

- In the PAVT the second most important parameter was by the long-term permeability of an intrusion borehole (BHPERM). The two parameters, TAUFAIL and BHPERM, are important because the total normalized release of radioactive material is dominated by cuttings and cavings and spallings. The shear strength affects cavings which is assumed to occur during every intrusion. The parameter BHPERM affects pressures in the repository, which in turns affects whether spallings would occur during an intrusion. In the PAVT, the BHPERM value of the lower end of the permeability range was lowered from  $10^{-14} \text{ m}^2$  to  $5 \times 10^{-17} \text{ m}^2$ . This caused more frequent pressures above 8 MPa than in the CCA PA, triggering more spallings events.
- EPA agreed with the Conceptual Model Peer Review Panel that the spallings conceptual model was inadequate but the results were reasonable for use in PA. EPA directed DOE to sample, in the PAVT, the CCA range of spallings releases (0.5 to 4.0 m<sup>3</sup>) when the repository pressure was greater than 8 Megapascals (Docket A-93-02, Item II-I-27). Eight megapascals is that pressure needed to overcome the hydrostatic pressure at the repository depth of 655 meters. This change in the modeling is captured in the new parameter VOLSPALL. When a spallings event occurred in the PAVT, the range for VOLSPALL, 0.5 to 4.0 m<sup>3</sup>, was sampled. In the CCA, the amount of spallings releases was determined by PARTDIA (CCA Appendix SA 3) when the pressure was greater than 8 megapascals.
- The PAVT and CCA modeled the same scenarios except that the 99% credit for passive institutional controls (PICs) was omitted in the PAVT. However, EPA's sensitivity analysis report (Technical Support Document for Section 194.23: Sensitivity Analysis Report, Docket A-93-02, Item V-B-13) and SNL impact analyses (WPO #41883 and WPO #41870) indicated that passive institutional controls are not important to releases. The effectiveness of PICs is due to the limited amount of time they are used (only 600 years beyond when credit for active institutional controls ends).
- Another difference in the computations was that, in the PAVT, the disturbed rock zone (DRZ) was allowed to fracture at lithostatic pressures, similar to the anhydrite. The effect of this was to prevent long-term unrealistic pressures to accumulate in the waste panel, because under increased pressure the DRZ will fail and fracture.
- The DRZ permeability parameter (DRZPERM) was constant in the CCA, but varied in the PAVT. In the Direct Brine Release Scenario DRZPERM was the most important parameter followed by the parameter for the initial brine pocket pressure (BPINTRS). In the CCA, brine saturation and halite porosity were the most important parameters (Docket A-93-02, Item II-G-30).
- In the PAVT, releases of brine were larger than in the CCA and the larger release volumes were due in part to an increase in waste permeability from  $1.7 \times 10^{-13} \text{ m}^3$  to  $2.4 \times 10^{-13} \text{ m}^3$ . (Section 6.1 of Docket A-93-02, Item II-G-28) Maximum volumes released in the PAVT

were 108 m<sup>3</sup>, 200 m<sup>3</sup>, and 105 m<sup>3</sup> in replicates 1 through 3, respectively. The maximum brine volume released in the CCA was 55 m<sup>3</sup>. This contributes to the greater releases from the direct brine release mechanism listed in Table 9. In addition, pressures in the undisturbed scenario, reached as high as 16.8 MPa in the PAVT compared to 16.3 MPa in the CCA.

- As in the CCA, the three PAVT replicates had very similar CCDFs. Figure 3, reproduced from Figure 7.1 of Docket A-93-02, Item II-G-28, is a graphical comparison of the CCA individual and mean curves and the PAVT individual and mean curves.

The change in parameters affected the different computational scenarios in the following manner (Docket A-93-02, Item II-G-28):

<u>Scenario</u>	<u>Parameters With Largest Effect on Listed Scenario in PAVT</u>
S1 Undisturbed Scenario	Corrosion rates and DRZ permeability, however, there was little effect from changes made for PAVT.
S2, S3 E1 intrusion at 350 and 1000 years	Brine reservoir volume, borehole permeability, corrosion rates
S4, S5 E2 intrusion at 350 and 1000 years	Corrosion rates, borehole permeability, and DRZ permeability
S6 E2 intrusion at 1000 years and an E1 intrusion at 2000 years	Brine reservoir volume, borehole permeability, corrosion rates

The parameters listed above affect pressure and brine saturation. For example, the lower range of long-term borehole permeability was reduced in the PAVT and this caused more high pressures in the repository. Also, the brine reservoir volume, increased in the BPINTRS parameter, increased brine availability for additional corrosion and related gas generation.

Table 9

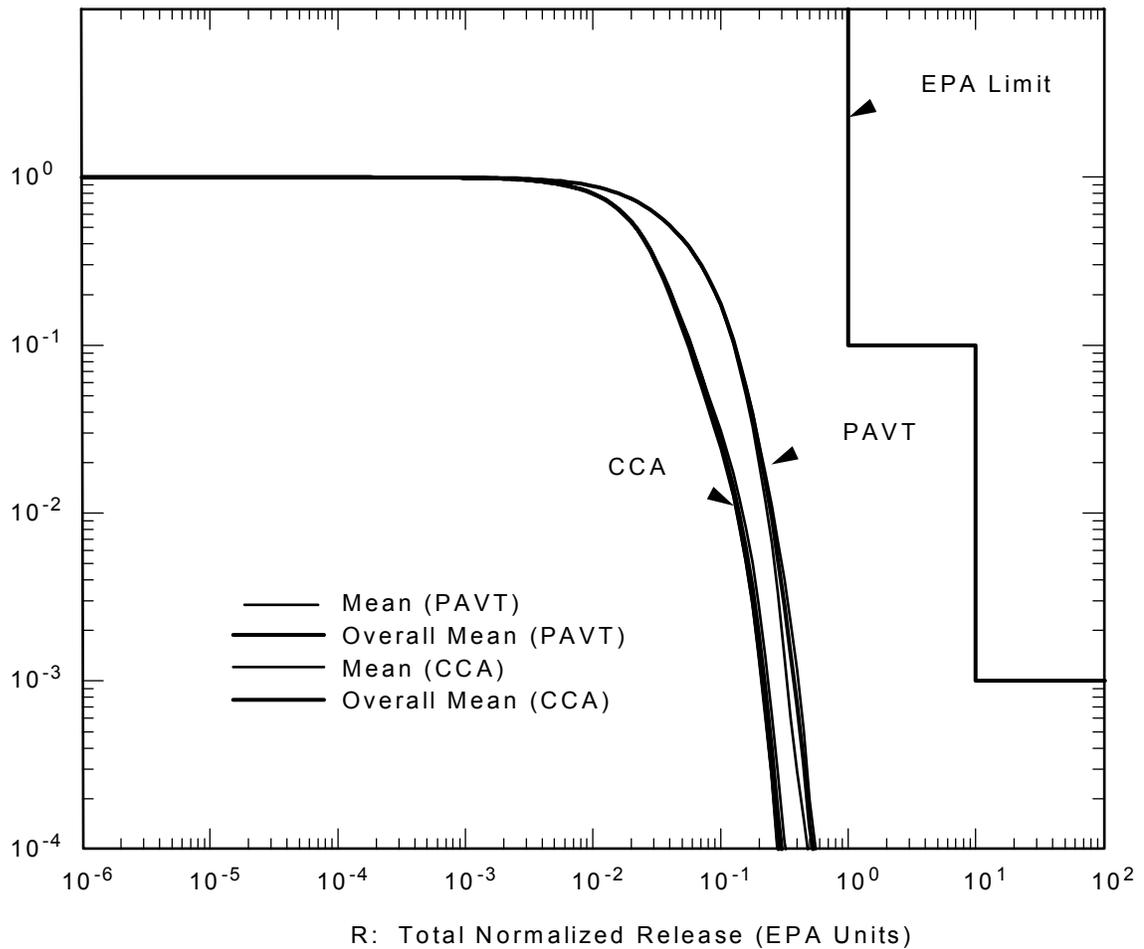
CCA and PAVT Normalized Releases for Probabilities of 0.1 and 0.001

Release Mechanism	EPA Units Released @ 0.1 Probability <sup>1</sup>		EPA Units Released @ 0.001 Probability <sup>1</sup>	
	PAVT	CCA	PAVT	CCA
Cuttings & Cavings	0.0732	0.0326	0.2754	0.1451
Spallings	0.0756	0.0310	0.2149	0.1750
Direct Brine Release	0.0003	0	0.1545	0.0452
Long-term Brine Release in the Culebra	0	0	0.0007	0
Total	0.1297 <sup>2</sup>	0.0576 <sup>2</sup>	0.3818 <sup>2</sup>	0.2219 <sup>2</sup>

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<sup>1</sup>Releases  $10^{-6}$  or less are considered to be zero.

<sup>2</sup>The releases from the individual release mechanisms do not sum to the total normalized release as may be expected. Because of the statistical nature of CCDF development, specifically the addition of random variables, the summary curves are not additive. The document “Distributions of Sums of Random Variables (WPO #47451) illustrates why this is the case. The summary curves from the individual release mechanisms can, however, be compared between the CCA and the PAVT.



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Note: Four CCDFs are shown for both the CCA and PAVT, including three individual mean CCDFs calculated for each of the three distributions of CCDFs calculated for the three replicates and an overall mean CCDF that is the arithmetic mean of the three individual mean CCDFs.

Figure 3: Comparison of Mean CCDF Curves Resulting from CCA PA and PAVT.

(After Figure 7.1 of DOE Document WPO #46702; see EPA Docket A-93-02, Item II-G-28.)

Table 10

## Parameters Used in the EPA-Mandated Performance Assessment

ID No.	Material	Parameter	Distribution Type/Unit	Min	Max	Med	Mean	Standard Dev.
198	DRZ_1	PRMX_LOG	Loguniform/m <sup>2</sup>	3.98E-20	3.16E-13	1.12E-16	1.99E-14	5.24E-14
3184	BH_SAND	PRMX_LOG	Loguniform/m <sup>2</sup>	5.01E-17	1.00E-11	2.24E-14	8.19E-13	7.85E-12
8001	CONC_PLG	PRMX	Uniform/m <sup>2</sup>	1.0E-19	1.0E-17	5.05E-18	--	--
663	WAS_AREA	PRMX_LOG	Constant/m <sup>2</sup>	2.4E-13	2.4E-13	2.4E-13	2.4E-13	0.00
2131	REPOSIT	PRMX_LOG	Constant/m <sup>2</sup>	2.4E-13	2.4E-13	2.4E-13	2.4E-13	0.00
2907	STEEL	CORRMCO2	Uniform/ M/S	0.00	3.17E-14	1.585E-14	1.585E-14	9.151E-15
61	CASTILER	COMP_RCK	Triangular/log (Pa <sup>-1</sup> )	2.00E-11	1.00E-10	4.00E-11	5.333E-11	1.6997E-11
3493	GLOBAL	PBRINE	Uniform/None	0.01	0.60	0.305	0.305	0.1703
27	BOREHOLE	DOMEGA	Cumulative/ rad/s	4.20	23.0	7.77	8.63	3.16
3482	AM+3	MKD_AM	Loguniform/ m <sup>3</sup> /kg	0.020	0.500	0.100	0.1491	0.1286
3480	PU+3	MKD_PU	Loguniform/ m <sup>3</sup> /kg	0.020	0.500	0.100	0.1491	0.1286
3481	PU+4	MKD_PU	Loguniform/ m <sup>3</sup> /kg	0.900	20.0	4.243	6.1591	5.141
3479	U+4	MKD_U	Loguniform/ m <sup>3</sup> /kg	0.900	20.0	4.243	6.1591	5.141
3475	U+6	MKD_U	Loguniform/ m <sup>3</sup> /kg	3.00E-5	3.00E-2	9.487E-4	4.339E-3	6.808E-3
3406	SOLMOD3	SOLSIM	Constant/ moles/liter	1.2E-7	1.2E-7	1.2E-7	1.2E-7	0.00
3402	SOLMOD3	SOLCIM	Constant/ moles/liter	1.3E-8	1.3E-8	1.3E-8	1.3E-8	0.00
3407	SOLMOD4	SOLSIM	Constant/ moles/liter	1.3E-8	1.3E-8	1.3E-8	1.3E-8	0.00
3403	SOLMOD4	SOLCIM	Constant/ moles/liter	4.1E-8	4.1E-8	4.1E-8	4.1E-8	0.00

ID No.	Material	Parameter	Distribution Type/Unit	Min	Max	Med	Mean	Standard Dev.
3408	SOLMOD5	SOLSIM	Constant/ moles/liter	2.4E-7	2.4E-7	2.4E-7	2.4E-7	0.00
3404	SOLMOD5	SOLCIM	Constant/ moles/liter	4.8E-7	4.8E-7	4.8E-7	4.8E-7	0.00
3478	TH+4	MKD_TH	Loguniform/ m3/kg	0.900	20.0	4.243	6.1591	5.141
2254	BOREHOLE	TAUFAIL	Loguniform/Pa	0.05	77	--	--	--
8004	WAS-AREA	VOL SPALL	Uniform/m <sup>3</sup>	0.50	4.00	2.25	2.25	1.01

Table 11

Parameters With Major Effects on Individual Release Mechanisms<sup>3</sup>

<u>Release Mechanism</u>	<u>CCA Parameter</u>	<u>PAVT Parameter</u>
Cuttings	WTAUFAIL	WTAUFAIL
Spallings	WMICDFLG	BHPRM, VOLSPALL, WMICDFLG
DBR	WRBRNSAT, HALPOR	DRZPRM, BPINTPRS
Culebra (U-234)	BHPRM, BPCOMP	BHPRM

(Table derived from Docket A-93-02, Item II-G-30 PAVT Uncertainty and Sensitivity Analysis)

Parameter Definitions from Docket A-93-02, Item II-G-30

WTAUFAIL	Waste erosion shear resistance for cavings
WMICDFLG	Flag parameter for gas generation
BHPRM	Long-term intrusion borehole permeability
VOLSPALL	Volume of spallings released; between 0.5 cubic meters and 4.0 cubic meters when repository pressure > 8 MPa, otherwise the value is 0 cu. meters; used only in PAVT
WRBRNSAT	Brine saturation of repository waste
HALPOR	Salado halite porosity
DRZPRM	Permeability of disturbed rock zone; sampled in PAVT, constant in CCA calculations
BPINTPRS	Initial pressure of Castile brine pocket
BPCOMP	Castile brine pocket compressibility

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<sup>3</sup>Some of the parameters have slightly different notations here than in the rest of the document. Document Docket A-93-02, Item II-G-30 uses a different nomenclature than most other DOE documents.

Table 12

Reproduced from Docket A-93-02, Item II-G-30, Table 6.1.1  
 Stepwise Regression Analysis with Rank-Transformed Data for Expected Normalized Release  
 Associated with Individual CCDFs for Total Release Due to Cuttings, Spallings, and Direct Brine  
 Release from the PAVT

	Expected Normalize Release		
Step <sup>a</sup>	Variable <sup>b</sup>	SRRC <sup>c</sup>	R <sup>2</sup> <sup>d</sup>
1	WTAUFAIL	-0.61	0.39
2	BHPRM	-0.40	0.56
3	VOLSPALL	0.33	0.66
4	WMICDFLG	0.27	0.74
5	HALPOR	0.13	0.76
6	DRZPRM	0.12	0.78
7	PRBRINE	0.12	0.79

- a Steps in stepwise regression analysis.
- b Variables listed in order of selection of regression analysis.
- c Standardized regression coefficients in final regression model with ANHCOMP and HALCOMP excluded from entry into regression model.
- d Cumulative R<sup>2</sup> value with entry of each variable into regression model.

## 6.0 Conclusions

DOE submitted the Compliance Certification Application to EPA for approval. A large part of the CCA involves the use of computers to evaluate the movement of radionuclides within the disposal system. The WIPP computer modeling is based on a conceptualization of site characteristics and potential future processes that may occur at the site, such as waste interactions, human intrusion, and creep closure of the salt. The characterization activities, the identification of the processes, and the modeling of those processes constitute PA. The PA, in turn, provides information on whether WIPP can contain radionuclides as required in the disposal regulations at 40 CFR 191.13.

DOE identified 24 major conceptual models that use site characterization and related information to capture those elements of the site that are believed to affect the performance of WIPP. DOE's evaluation work, previous PAs and the CCA have shown that some of these conceptual models are more important than others in determining how well the WIPP can contain radionuclides. The most important of the processes that may affect WIPP's ability to contain radionuclides are related to human activity: 1) cuttings and cavings, 2) spillings, and 3) direct brine releases. The human intrusion case (multiple boreholes drilled into the same panel) that could provide the most releases has a low probability. The fourth potential release mechanism is long-term brine release through the Culebra dolomite and the Salado anhydrite markerbeds; however, this pathway contributes very little to releases. It is expected that there will be no disruptive events, such as earthquakes, and radionuclides are expected to remain in the repository. One aspect related to human activity that had little affect on releases was credit for passive institutional controls, in large part due to the short time they were assumed to be effective. In addition, fluid injection related to oil production is not considered to adversely affect the WIPP and has been appropriately screened out.

EPA conducted verification modeling for spillings, radionuclide transport in groundwater, actinide solubility, and general parameter sensitivity modeling. EPA's spillings modeling used bounding assumptions, such as no mud in the drilling borehole and lack of waste strength, and identified that the spillings model used by DOE overestimates the volume of material expected to be released from a spill event. EPA's ground-water modeling verifies DOE's contention that even small amounts of chemical retardation are effective in reducing radionuclide transport in the Culebra. EPA's actinide solubility review and modeling indicated that the solubility values used in the CCA were higher than that expected by EPA. In reviewing DOE's parameters, EPA conducted an extensive review that included independent sensitivity analyses as well as confirmatory modeling (such as the ground-water modeling of chemical retardation).

EPA reviewed DOE's parameter development process and identified that DOE had a great deal of documentation available on the parameters, however, EPA identified a small percentage of parameters that were questionable. Of the 58 parameters questioned by EPA, many were resolved with additional documentation. Twenty-four parameters remained in questioned and were changed for the PAVT. In addition, EPA identified issues related to coding errors for several computer codes. In responding to EPA's issues, DOE discovered and rectified

several minor coding errors. Results from an impact analysis by DOE indicated that the coding errors would have had very little impact on PA results. These issues were resolved to EPA's satisfaction.

EPA directed DOE to demonstrate the combined effect of the parameter and code changes by conducting additional calculations in a PAVT. The PAVT was an independent computer simulation of the WIPP's performance conducted under EPA's authority to require independent verification computer simulations (§194.23(d)). The PAVT resulted in 300 CCDF curves that verified that the combined effect of computer code changes and altered parameter values did not significantly alter the results of the PA and did not cause the predicted releases from the WIPP to violate the containment requirements. The CCDF curves show slightly higher normalized releases than the CCA PA, but they are still much below the radioactive waste containment requirements at §191.13. The PAVT incorporated changes that addressed EPA's concerns about the PA and demonstrated that the combined effect of the necessary modification did not require that DOE conduct a new full PA. Moreover, the results of the PAVT demonstrated that modeled resulting releases are still within the containment requirements. Because the PAVT used technical methods identical to those of the CCA PA, EPA believes that the PAVT results are numerically equivalent to those that would be obtained by performing a new PA that incorporated the same changes implemented in the PAVT. Therefore, because of the close agreement between the PA and PAVT results, EPA believes that the PAVT verifies that the original CCA PA was adequate for comparison against the radioactive waste containment requirements.

## 7.0 References

### References in EPA Air Docket A-93-02

- II-A-39      Chemical Conditions Model: Results of the MgO Backfill Efficacy Investigation
- V-B-2        CARD 14: Content of Compliance Application
- V-B-4        Technical Support Document for Section 194.14: Content of Compliance Application
- V-B-6        Technical Support Document for Section 194.23: Models and Computer Codes.
- V-B-7        Technical Support Document for Section 194.23: Groundwater Flow and Contaminant Transport Modeling at WIPP.
- V-B-12      Technical Support Document for Section 194.23: Parameter Report
- V-B-13      Technical Support Document for Section 194.23: Sensitivity Analysis Report
- V-B-14      Technical Support Document for Section 194.23: Parameter Justification Report
- V-B-17      Technical Support Document for Section 194.24: EPA's Evaluation of DOE's Actinide Source Term
- V-B-22      Technical Support Document for Section 194.32: Fluid Injection Analysis
- V-B-26      Technical Support Document for Section 194.55: Compliance Assessment Statistics
- V-C-1        Responses to Comments
- II-D-115     Letter from G. Dials to R. Neill, Attachment 2, Concerning Closeout of Issues concerning chemical retardation ( $K_d$ ) in the Culebra and including a summary of the July 30, 1997 meeting
- II-D-116     Bredehoeft, John and Walter Gerstle. The HARTMAN Scenario Revisited Implications for WIPP, August, 1997.
- II-D-118     Gerstle, Walter and John Bredehoeft, Linear Elastic Model for Hydrofracture at WIPP and Comparison with BRAGFLO Results, September 3, 1997
- II-G-8        Analysis Package for the Salado Flow Calculations (Task 1) of the Performance Assessment Analysis - WPO #40514, Supporting the Compliance Certification Application

- II-G-3                    Validation Document for CCDFGF
  
- II-G-22                Conceptual Model Peer Review Panel Third Supplementary Peer Review Report.
  
- II-G-26                Summary of EPA-Mandated Performance Assessment Verification Test (Replicate 1) and Comparison with the Compliance Certification Application Calculations
  
- II-G-28                Supplemental Summary of EPA-Mandated Performance Assessment Verification Test (All Replicates) and Comparison with the Compliance Certification Application Calculations - WPO#46702
  
- II-G-30                Summary of Uncertainty and Sensitivity Analysis Results for the EPA-Mandated Performance Assessment Verification Test - WPO #46912
  
- II-I-03                Larson et. al and Beauheim et al., 1994 in Letter from G. Dials (DOE) to R. Trovato (EPA) - second response package to EPA's letter of December 19, 1996 to DOE/A. Alm. Supplemental Information for the Compliance Certification Application (CCA).
  
- II-I-17                March 19, 1997 Letter from R. Trovato (EPA) to A. Alm (DOE), transmitting comments regarding completeness and technical sufficiency of DOE's Compliance Certification Application w/6 Enclosures.
  
- II-I-24                April 15, 1997 Letter from G. Dials (DOE-CAO) to R. Trovato (EPA), responding to March 19, 1997 letter to A. Alm regarding CCA issues/comments.
  
- II-I-27                Letter from EPA/R. Trovato to DOE/CAO/G. Dials, follow-up to EPA Letter of March 19, 1997 to DOE/A. Alm regarding Performance Assessment input parameters
  
- II-I-55                August 27, 1997 letter: George Dials to Lawrence Weinstock, Evaluation of the Equivalency of the CCA Performance Assessment and the EPA Mandated Performance Assessment Verification Test
  
- II-I-36                Letter from DOE/CAO/G. Dials to EPA/L. Weinstock responding to EPA's letter of March 19, 1997 requesting additional information regarding water flooding. Item b, Sandia National Laboratories - Waste Isolation Pilot Plant - ExpeditedCCA Activity - WPO #44158 Supplementary Analyses of the Effect of Salt Water Disposal and Waterflooding on the WIPP.

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WPO #47451 Froehlich, G. K, October 3, 1997, Distributions of Sums of Random Variables.

WPO #46936 Estimate WIPP Waste Particle Size on Expert Elicitation Results: Revision 1", August 5, 1997 memorandum from Yifeng Want to Margaret Chu.

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WPO #23378 Beauheim, R.L., Roberts, R.M., Dale, T., Fort, M.D., and Strensrud, W.A. 1993. Hydraulic Testing of Salado Formation Evaporites at the Waste Isolation Pilot Plant Site: Second Interpretive Report. SAND92-0533, Sandia National Laboratories, Albuquerque, NM.