

CARD No. 23

Models and Computer Codes

23.A BACKGROUND

Section 194.23 addresses the compliance criteria requirements for conceptual models and computer codes. Conceptual models capture a general understanding of the disposal system and are used as the basis for computer simulations of how well the disposal system will contain radionuclides. Results of the analysis of the disposal system's performance are incorporated into numerical comparisons with the containment requirements of Section 191.13.

DOE identified relevant features, events, and processes (FEPs) that might affect the disposal system and then created models, or theories, to describe the characteristics of the WIPP and the potential for radionuclides to be contained. The individual processes and events are grouped into "scenarios." These processes and events were used by DOE to develop 24 major "conceptual models" for inclusion in the WIPP performance assessment (PA).

The design of computer codes begins with the development of conceptual models. Conceptual models consider the design of the repository and the FEPs that may occur at the WIPP that could lead to the retention or release of radionuclides. In order for the final computer codes to obtain realistic solutions, the underlying conceptual models must be sound. DOE must next develop mathematical models from the conceptual models. Mathematical models set up a mathematical expression to describe the conditions in the repository and its surroundings. Examples of mathematical models that represented scenarios and conceptual models are fluid flow in the repository and surrounding formations, mechanical deformation of halite, and radionuclide transport in the repository and overlying rock formations. Numerical models are then created to describe how to solve the equations in the mathematical models. Since most of the mathematical models are sufficiently complex that unique solutions are not possible, numerical models are used to provide iterative, approximate solutions to the mathematical models. Finally, DOE must program the numerical solutions from the numerical models into computer codes that calculate the estimated cumulative releases of radionuclides caused by all significant processes and events.

The Compliance Criteria at Section 194.23 impose significant requirements on the development and presentation of conceptual models and computer codes that are used to demonstrate that the WIPP will comply with the radioactive waste disposal regulations at 40 CFR Part 191. Section 194.23(a) requires descriptions of conceptual models and scenario construction; consideration of alternative conceptual models; documentation that conceptual models and scenarios reasonably represent possible future states of the disposal system, mathematical models reasonably represent the conceptual models, and numerical models (or solution methods) provide stable solutions to the mathematical models; and that DOE organize a peer review of conceptual models. Section 194.23(b) requires that computer codes be documented in accordance with a proper quality assurance methodology. Section 194.23(c) requires: documentation of all models and computer codes; detailed descriptions of data collection, data reduction and analysis, and parameters developed from source data; detailed descriptions of the structure of the computer codes; and a complete listing of source codes.

This CARD summarizes the criteria used by EPA to evaluate DOE's compliance with the requirements of Section 194.23, the approach taken by DOE to address each requirement as documented in the CCA and other supporting documents, and significant aspects of EPA's review of DOE's approach. Detailed discussions of specific aspects of EPA's compliance review may be found in EPA Technical Support Documents referenced by this CARD. Section 17.0 of this CARD ("References in Air Docket A-93-02") contains reference information for docket items cited in the text.

1.0 REQUIREMENT

(a) "Any compliance application shall include:

(1) A description of the conceptual models and scenario construction used to support any compliance application."

1.1 ABSTRACT

DOE developed 24 conceptual models to describe the WIPP disposal system. DOE also undertook an extensive screening process to determine which FEPs were applicable to the disposal system. From the list of applicable FEPs, DOE developed scenarios to describe both undisturbed and disturbed performance (human intrusion) of the repository. Scenarios were included that satisfy the specific requirements of Sections 194.32 and 194.33 of the Compliance Criteria. Refer to **CARD 32—Scope of Performance Assessments and CARD 33—Consideration of Drilling Events in Performance Assessments**. EPA reviewed the descriptions of the conceptual models and the scenario construction methods in the CCA and supplementary information and found them to be complete, accurate, and presented with sufficient clarity to permit full understanding of the descriptions and methods. Additional information supporting EPA's proposed decision is provided in Section 1 of the EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6).

1.2 COMPLIANCE REVIEW CRITERIA

EPA expected the CCA to contain a complete, clear, and logical description of each of the conceptual models used. Documentation of the conceptual models should discuss site characteristics and other characteristics such as processes active at the site (e.g., gas generation or creep closure of the Salado salt formation). The conceptual models should represent those characteristics and attributes of the WIPP disposal system that adequately describe the performance of the disposal system. In other words, the conceptual models should be appropriate simplifications of the characteristics, attributes, and processes that describe the disposal system. The conceptual models should consider both natural and engineered barriers.

The CCA should contain a complete and logical description of the scenario construction methods used. The scenario construction descriptions should include sufficient detail to understand the basis for selecting certain scenarios and rejecting others. Descriptions should be presented in a clear and understandable manner to reduce the possibility of misinterpretation.

1.3 DOE METHODOLOGY AND CONCLUSIONS

1.3.1 Location of Information in the CCA

Summary information on conceptual models and scenario construction is included in particular on p. 6-3, p. 6-16, p. 6-24, p. 6-29, p. 6-40, p. 6-61, p. 6-71, p. 6-77, p. 6-78, p. 6-203, and p. 6-204 of the CCA (Docket A-93-02, Item II-G-1). A number of CCA appendices provide specific information in support of Chapter 6 of the CCA, including descriptions of the computer codes used to implement these models and to characterize the consequences of the developed scenarios, the assumptions made in screening various scenarios to be included or excluded in the PA, the parameters used in the codes, and the sensitivity of the modeling results to parameter assumptions. These appendices are described in Table 1-6, pp. 1-28 to 1-30 of the CCA.

Substantial additional information is included in the original Conceptual Model Peer Review Panel (CMPRP) Report (CCA Appendix PEER.1); DOE's initial response to the July 1996 CMPRP Report (Chapter 9, pp. 9-9 to 9-120); and the CMPRP's first, second, and third supplementary reports, which were provided by DOE as supplements to the CCA and placed in the docket (Docket A-93-02, Items II-G-12, II-G-21, and II-G-22, respectively). For a discussion of the Conceptual Model Peer Review, see Section 7.0 of this CARD.

1.3.2 DOE's Methodology

1.3.2.1 Scenario Construction

DOE's methodology for scenario construction is driven by the containment requirements of Section 194.13, which specify that based on PAs, cumulative releases to the accessible environment during 10,000 years must meet certain probability conditions. PA is defined as an analysis that:

- ◆□ Identifies the processes and events that might affect the disposal system.
- ◆□ Examines the effects of these processes and events on the performance of the disposal system.
- ◆□ Estimates the cumulative releases of radionuclides, considering the associated uncertainties, caused by all significant processes and events (see 40 CFR 191.12.)

For consistency with this regulatory definition, DOE developed a process to identify and screen processes and events and combine them into scenarios. This process consisted of the following steps:

- ◆ □ FEPs potentially relevant to the WIPP were identified and classified.
- ◆ □ Defined screening criteria were used to eliminate certain FEPs as not important or relevant to the WIPP’s performance.
- ◆ □ Scenarios were formed from the remaining FEPs, in the context of regulatory requirements for developing performance criteria.
- ◆ □ Scenarios were specified for consequence analysis, as part of PA modeling (see Chapter 6, p. 6-29).

The FEPs screening process is described in Appendix SCR and is reviewed in detail in **CARD 32—Scope of Performance Assessments** and the EPA Technical Support Document for Section 194.32: Scope of Performance Assessment (Docket A-93-02, V-B-21). After the FEPs screening process identified the relevant processes and events, DOE selected scenarios—i.e., combinations of FEPs—for inclusion in the PA. DOE assembled the FEPs not eliminated by the screening process into undisturbed performance scenarios (natural processes and events) and disturbed performance scenarios (mining and deep drilling or human intrusion boreholes), based on the logic diagram (p. 6-63, Figure 6-7) reproduced in Figure 1 of this CARD.

Undisturbed Performance Scenario

Undisturbed performance is defined in 40 CFR 191.12 as “the predicted behavior of a disposal system, including uncertainties in predicted behavior, if the disposal system is not disrupted by human intrusion or the occurrence of unlikely natural events.” As defined in Section 194.32, the undisturbed performance scenario includes the effects of human activities outside the controlled area. DOE identified 67 FEPs that were included in the undisturbed performance scenario. (See Table 6-6, pp. 6-65 to 6-68.) The human activities included in the undisturbed performance scenario outside the Land Withdrawal Boundary are potash mining and fluid injection related to hydrocarbon extraction.

According to DOE, brine in the Salado Formation is the only possible means of transporting radionuclides away from the disposal system in the undisturbed scenario. Any leakage of radioactive material to the accessible environment must involve brine that enters the repository, becomes contaminated with mobilized radionuclides, and leaves the repository by one or more of several possible pathways. Pathways described by DOE in Appendix DEF include:

- ◆ Lateral flow through the waste storage regions and vertical flow upward along failed shaft seals to the land surface.
- ◆ Lateral flow through the waste storage regions, vertical flow upward along failed shaft seals, and lateral flow through the Culebra dolomite (or other transmissive unit) to the subsurface WIPP site boundary.

- ◆ □ Leakage through the disturbed rock zone (DRZ), around the WIPP excavation, and into underlying anhydrite marker bed MB-139, and lateral flow to the subsurface WIPP site boundary.

This topic is also discussed in **CARD 14—Content of Compliance Certification Application**. In each case, sufficient pressure must exist in the repository to provide the driving force for brine migration. DOE stated that direct leakage through the Salado halite is not possible because of the low permeability of the undisturbed halite.

Disturbed Performance—Drilling

Section 194.33 requires that PAs examine shallow and deep drilling that might affect the disposal system. See **CARD 33—Consideration of Drilling Events in Performance Assessments**. DOE excluded shallow drilling (i.e., no deeper than 2,150 feet) on the basis of low consequence (Chapter 6.2.5.2, pp. 6-58 to 6-61). Deep drilling was included in the PA. Deep drilling is defined in Section 194.2 to mean “those drilling events in the Delaware Basin that reach or exceed a depth of 2,150 feet below the surface.” If a deep borehole intercepts waste, several release pathways are possible in addition to those in the undisturbed scenario.

DOE assumes that boreholes drilled in search of hydrocarbons pass through the Salado Formation and through the underlying Castile Formation (Appendix DEL.4.2.1 pp. DEL-10 to DEL-17). As discussed in the section on site characterization in the CCA (Chapter 2.1.3.3, pp. 2-24 to 2-29), pressurized brine reservoirs have been observed in the Castile formation and a borehole could intercept one of these brine pockets. Since a direct connection would exist between the pressurized brine pocket and waste, a drilling event that intersects both brine and waste could enhance waste transport from the repository to the surface. DOE designated a scenario in which a borehole intersects both waste in the repository and a Castile brine pocket reservoir as an E1 scenario (Chapter 6.3.2.2.2, p. 6-77).

Depending on the extent to which the repository is underlain by brine pocket reservoirs, a borehole which penetrates a waste panel may not intersect a Castile brine pocket reservoir. DOE defines a deep drilling scenario where waste is intersected, but a Castile brine pocket is not intersected, as an E2 scenario (Chapter 6.3.2.2.2, p. 6-77).

It is possible that multiple intrusions could occur in the same waste panel during the 10,000 year regulatory time frame. To address this possibility, DOE defines an E1E2 scenario as one in which multiple intrusions occur in the same waste panel and at least one scenario is an E1 (Chapter 6, pp. 6-77 to 6-78). Many versions of the E1E2 scenario are possible depending on intrusion time, drilling sequence, and location of the borehole within the waste panel. The E1E2 scenario, which results in a potential flow path through all the waste in a panel, can create the opportunity for larger amounts of radioactive contamination to be mobilized and transported out of the repository, which enhances the potential release.

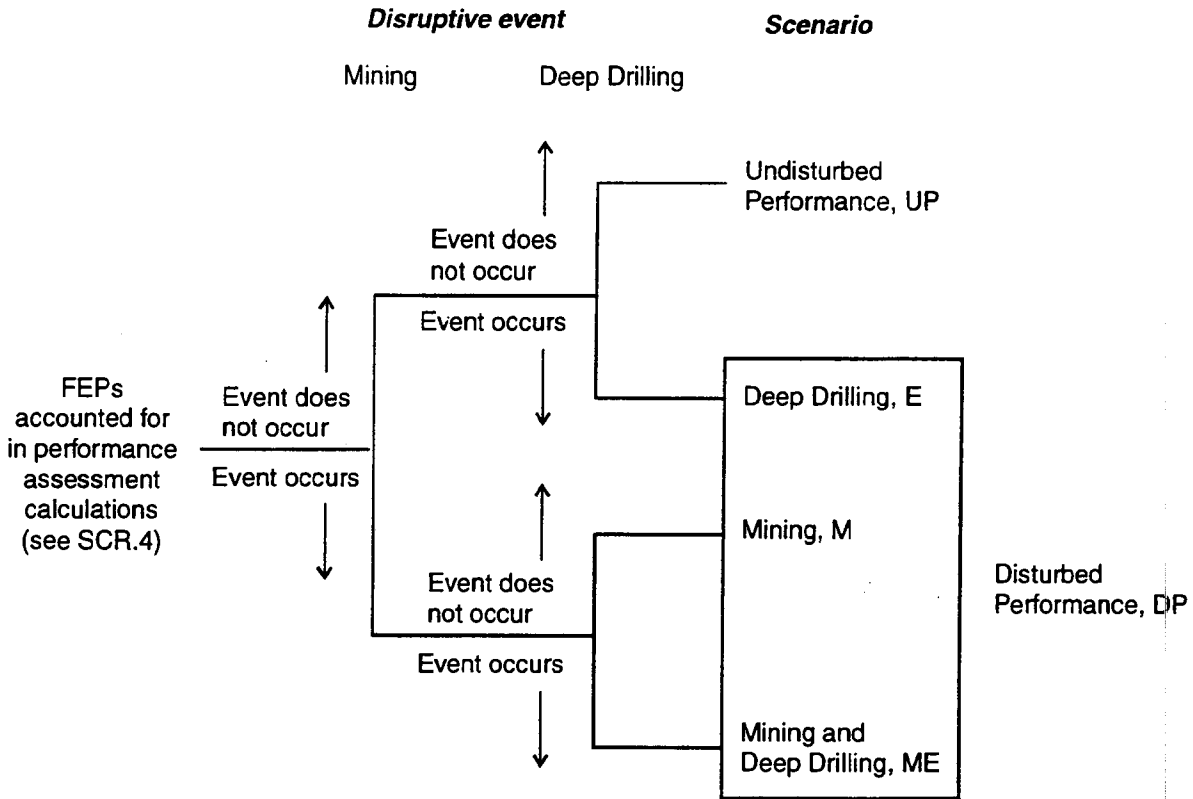
Deep drilling can create several pathways (e.g., direct releases to the surface and potential release to more shallow formations, such as the Rustler Culebra member above the WIPP site) by which radioactive contamination can reach the accessible environment if waste is intersected by a

borehole. These pathways can augment releases categorized as either short-term or long-term. Short-term releases occur over a few days at most and are described by the cuttings/cavings, spillings, and direct brine release conceptual models. For examples, see EPA's discussion of these models in Sections 1.3.4, 1.3.5, and 1.3.9 of EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6). Long-term releases from deep drilling scenarios involve flow and transport through transmissive units above the Salado, where the borehole(s) provides the hydraulic connection between the repository and the overlying units. See, for example, EPA's discussion of Culebra hydrogeology, transport of dissolved actinides in the Culebra, and transport of colloidal actinides in the Culebra in Sections 1.3.17, 1.3.18, and 1.3.19 of the EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6). Deep boreholes that intersect waste can also hit brine pocket reservoirs in the Castile Formation underlying the repository. Under the multiple intrusions conceptual model, brine reservoirs are assumed to be depleted if intercepted by multiple boreholes, with the number of boreholes required to cause depletion determined by the size of the reservoir (Chapter 6.4.12.6, pp. 6-190 and 6-198). If the number of intrusions is less than that required for reservoir depletion, reservoir properties are maintained within the assumed parameter distributions throughout the 10,000 year regulatory time frame (Chapter 6.4.12.6, p. 6-198).

The probability that the waste will be intersected by a borehole is modeled as a Poisson process¹, with a rate constant determined from the historic drilling rate in the Delaware Basin of 46.8 boreholes per square kilometer per 10,000 years (p. 6-182). With 0.126 km² as the area in the panels containing waste, the Poisson rate constant is 5.9×10^{-4} boreholes per year. This drilling rate is assumed to remain constant for the period from 700 to 10,000 years after disposal. However, DOE set the drilling rate constant at 5.9×10^{-6} for the period from 100 to 700 years based on assumed credit for passive institutional controls, and DOE set the rate at zero for the first 100 years based on the assumption of complete deterrence of active institutional controls (Chapter 6.4.12.2, pp. 6-182 to 6-183). See **CARD 41—Active Institutional Controls** for a discussion of the basis for active institutional controls' effect on the drilling rate. See **CARD 43—Passive Institutional Controls** for a discussion of the basis for passive institutional controls' effect on the drilling rate.

Using the Poisson model, DOE calculated the most likely number of boreholes hitting waste to be five, with a probability of occurrence of 0.1715. The probability of zero boreholes intersecting waste is 0.0041. The maximum number of intrusions with a probability of greater than 10^{-3} (0.001) is 14 (p. 6-183). (The probability of 0.001 is important because it is the value of the lower probability requirement in Section 191.13(a)(2).) Boreholes may: a) intercept brine, b) intercept waste, c) intercept brine and waste, or d) intercept neither brine nor waste. If the borehole encounters waste, there is an immediate direct release of cuttings and cavings to the

¹ A Poisson process is random in time and obeys a mathematical formula. It may be used to predict the probability of a particular event over time, if one knows the rate constant for the average number of events per time. DOE discusses the use of a Poisson process for estimating the number and time of drilling intrusions in Chapter 6, pp. 6-182 and 6-183. In the case of the CCA, the particular event is the drilling of a borehole, and the rate constant is the historic drilling rate over the 100 years before the CCA was submitted in boreholes per year, as required by 194.33(b)(3)(i) (see **CARD 33—Consideration of Drilling Events in Performance Assessments**).



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Figure 1: Logic Diagram for Scenario Analysis

surface because of the direct action of the drill bit. If the repository pressure exceeds 8 MPa, there can also be spallings solid releases and direct brine releases. If the borehole hits a Castile brine pocket, there can be long term releases via lateral transport to the accessible environment or direct releases from subsequent borehole intrusions. If neither brine nor waste are intercepted, the intrusion is assumed to have no impact (Chapter 6.4.12.6, p. 6-198).

Disturbed Performance—Mining

Section 194.32(a) of the Compliance Criteria requires that PAs consider mining, and Section 194.32(b) identifies the manner in which mining should be considered:

Assessments of mining effects may be limited to changes in the hydraulic conductivity of the hydrogeologic units of the disposal system from excavation mining for natural resources. Mining shall be assumed to occur with a one in 100 probability in each century of the regulatory time frame. PAs shall assume that mineral deposits of those resources, similar in quantity and type to those resources currently extracted from the Delaware Basin, will be completely removed from the

controlled area during the century in which mining is randomly calculated to occur. Complete removal of such resources shall be assumed to occur only once during the regulatory time frame.

As shown in the logic diagram of Figure 1 above, mining can occur either with or without the occurrence of deep drilling.

DOE evaluated the time at which the mining scenario occurs in PA in the CCDFGF computer code, using a Poisson random model methodology and a probability of 10^{-4} intrusions per year (and 10^{-6} per year during the period of assumed effectiveness for passive institutional controls). The mining scenario was assumed to involve removal of potash from the Salado Formation above the repository which causes subsidence of the overlying units. Subsidence can produce fracturing in the more brittle rock strata above the potash mining zone which can be modeled by increasing the hydraulic conductivity of units above the potash zone mined. Modeling of the mining scenario is similar to modeling the undisturbed case, except that the hydraulic conductivity of the Culobra is altered due to assumed subsidence-induced fracturing (Chapter 6, p. 6-71). Hydraulic conductivity of mined areas is up to one thousand times that of areas that are not mined.

Computational Scenarios Included

DOE constructed six scenarios in the PA calculations, denoted S1 to S6 (Chapter 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 to 59). These six computational scenarios used in the PA calculations are as follows:

- ◆ □ S1—the undisturbed scenario.
- ◆ □ S2—an E1 scenario in which a borehole passes through the waste and into a Castile brine pocket at 350 years.
- ◆ □ S3—an E1 scenario in which a borehole passes through the waste and into a Castile brine pocket at 1000 years.
- ◆ □ S4—an E2 scenario in which a borehole passes through the waste and misses the Castile brine pocket at 350 years.
- ◆ □ S5—an E2 scenario in which a borehole passes through the waste and misses the Castile brine pocket at 1000 years.
- ◆ □ S6—an E2E1 scenario in which two boreholes pass through the waste: one that misses the Castile brine pocket at 1000 years and one that drills into a Castile brine pocket at 2000 years.

The first of these six scenarios is the undisturbed case, while the other five are disturbed scenarios in which human intrusion occurs. The time of intrusion calculated in scenarios S2-S6 was selected so that gas generation impacts would be at their greatest. The consequences of

these scenarios are calculated by using a series of computer codes that implement the appropriate conceptual models, as discussed in the background to this CARD.

1.3.2.2 Conceptual Model Description

DOE defines conceptual models as “a set of qualitative assumptions used to describe a system or subsystem for a given purpose. At a minimum these assumptions concern the geometry and dimensionality of the system, initial and boundary conditions, time dependence, and the nature of the relevant physical and chemical processes” (Chapter 6, p. 6-85).

Summary discussion of the conceptual models used in the CCA and their integration into computer codes is presented in Chapter 6, and Volume X, Appendix MASS. Greater detail on many of the models is provided in the Analysis Packages that were supplied subsequent to the CCA submission (Docket A-93-02, Items II-G-04 to II-G-11). As discussed under Section 7.0 of this CARD, the Conceptual Models Peer Review Panel reviewed all the conceptual models to determine their adequacy for incorporation into the PA.

The 24 conceptual models included in the CCA are listed in Table 1 below. The components in this table refer to broad groupings of the conceptual models into those models related to human intrusion, to flow and transport within the Salado Formation, and to flow and transport in hydrostratigraphic units other than the Salado.

Table 1 lists the 24 conceptual models considered by the Conceptual Models Peer Review Panel. The component column lists the components of the conceptual modeling system to which each conceptual model applies. The conceptual models are discussed in Chapter 6.4 and Appendix PEER.1 of the CCA.

1.4 EPA COMPLIANCE REVIEW

DOE’s scenario construction process was based on screening decisions using a comprehensive list of FEPs developed for the Swedish Nuclear Power Inspectorate (SKI) and other WIPP-specific FEPs that were developed by DOE (see Chapter 6.2.1 of the CCA). DOE’s methodology for addressing conceptual model development and scenario construction consisted primarily of identifying and screening processes and events and combining them into scenarios. EPA reviewed each of the four steps that DOE used in this process as discussed in Section 1.3.2.1 above.

Table 1
WIPP Conceptual Models Used in CCA

Model	Component
1 Disposal System Geometry	Salado F/T ¹
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

¹ F/T - flow and transport.

EPA found that information documenting DOE's process of developing and identifying FEPs that are potentially relevant to the site and the scenarios that DOE developed from the selected FEPs to be generally thorough and complete (see also **CARD 32—Scope of Performance Assessments**, especially Section 32.A.5, for a discussion of FEPs at the WIPP site). However, DOE did not provide any discussion of the numerical implementation of precipitation or of colloidal preferential solubility. EPA required DOE to provide such information. EPA also required additional information on DOE's treatment of transport of colloids and radionuclides, filtration versus sorption, and the treatment of the Culebra as a fully confined system; see EPA's December 19, 1996, letter to DOE (Docket A-93-02, Item II-I-01). DOE addressed EPA's questions with further documentation (Docket A-93-02, Items II-I-03, II-I-07, and II-I-16).

In addition, EPA challenged various initial DOE assumptions used to screen out oil production related fluid injection (for brine disposal and secondary oil recovery) on the basis of low consequence. See EPA's March 19, 1997, letter to DOE (Docket A-93-02, Item II-I-17). EPA determined that DOE had not performed sufficient analyses to rule out the potential effects of fluid injection on the disposal system. Therefore, EPA required DOE to perform additional analyses of fluid injection (Docket A-93-02, Item II-G-25, Sandia National Laboratories - Supplementary Analyses of the Effect of Salt Water Disposal and Waterflooding on the WIPP; Docket A-93-02, Item V-B-22, Technical Support Document for Section 194.32: Fluid Injection Analysis (Section 4.0); and Docket A-93-02, Item V-B-6, Section 1.2.2.2 of EPA Technical Support Document for Section 194.23: Models and Computer Codes). Based on its analysis of supplementary information provided by DOE, EPA now believes that fluid injection can be screened out from the PA as a result of the additional evaluations performed by DOE. A detailed discussion of fluid injection and relevant documentation may be found in **CARD 32—Scope of Performance Assessments**, especially section 32.C.5.

Upon reviewing models and computer codes, EPA found that certain of the conceptual models utilized in the derivation of certain input parameters were changed by DOE or its contractors after submission of the CCA. EPA also questioned a number of important input parameter values and distributions used in the PA. In addition, EPA found DOE's justification of credit for 99 percent effectiveness of passive institutional controls (PICs) to be insufficient. Because of concerns that the necessary corrections to these input parameters and conceptual models and the removal of the credit for PICs could have significant effects on the actual results of the PA, EPA required DOE to demonstrate that the combined effect of all the parameter and computer code changes required by EPA was not significant enough to necessitate a new PA (Docket A-93-02, Item II-I-17). EPA directed DOE to demonstrate the combined effect of the parameter and code changes by conducting additional calculations in a Performance Assessment Verification Test (PAVT). The PAVT implemented DOE's PA modeling, using the same sampling methods as the PA, but incorporating parameter values mandated by EPA and eliminating the credit for PICs (Docket A-93-02, Items II-I-25 and II-I-27).

Refer to **CARD 32—Scope of Performance Assessments**, especially section 32.B, for a discussion of mining scenarios, a review of FEPs used to construct scenarios, and intrusion scenarios assumed to occur before disposal. Refer to **CARD 33—Consideration of Drilling Events in Performance Assessments**, especially section 33.A, for information on drilling scenarios used in the development of the PA conceptual models.

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 peer review panel that all models except the spallings model were adequate for use in the PA calculations. The Conceptual Models Peer Review Panel initially 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 (see Sections 2.0 and 7.0 of this CARD for further discussion). However, the peer review panel ultimately found that the results from the spallings model are reasonable and that they may even overestimate releases (Docket A-93-02, Item II-G-22, p. 17). 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 up to 10 times or more (Spallings Release Position Paper, Docket A-93-02, II-G-23).

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.

EPA concluded that the CCA contains an adequate description of the scenario construction methods used, and that the scenario construction descriptions include sufficient detail to understand the basis for selecting some scenarios and rejecting others. Further discussion of the conceptual models and the review process, including EPA's consideration of supplementary information, is included in Section 1.2 of EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6).

During the public comment period on EPA's proposed certification decision, the Agency received comments related to many aspects of DOE's conceptual models. These included comments on DOE and EPA's treatment of spallings and DOE's decision to model only the "blowout" spallings mechanism and not "stuck pipe" or "gas erosion" mechanisms. Commenters stated that DOE should have included additional scenarios of human intrusion in performance assessment, including fluid injection, air drilling, CO₂ injection, and solution potash mining. Commenters also stated that certain aspects of WIPP geology should be modeled differently.

In response to issues raised by commenters, the Agency completed an additional analysis of the impact of air drilling, carbon dioxide injection, and fluid injection on the WIPP. See EPA's Analysis of Air Drilling at WIPP (Docket A-93-02, Item V-B-29), the CO₂ Injection discussion in the Response to Comment, Section 8, and the Fluid Injection section of the Response to Comment, Section 5 (Docket A-93-02, Item V-C-1). For a general discussion of these issues and EPA's responses, see the "Modeling and Performance Assessment" section of the preamble. For a detailed discussion of these issues, see the Response to Comments Document.

2.0 REQUIREMENT

(a) "Any compliance application shall include:

(2) A description of plausible, alternative conceptual model(s) seriously considered but not used to support such application, and an explanation of the reason(s) why such model(s) was not deemed to accurately portray performance of the disposal system."

2.1 ABSTRACT

DOE provided a description of plausible alternative conceptual models considered but not used in the PA in the CCA and supplementary information. DOE also explained the reasons why these alternative models were not used to describe the performance of the repository. EPA evaluated the technical adequacy of DOE's explanation of why plausible, alternative conceptual models were not used. Additional discussion of EPA's review and detailed references to the CCA and supplementary information may be found in Section 2.0 of EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6).

2.2 COMPLIANCE REVIEW CRITERIA

The CCA should contain a description of the plausible alternative conceptual models considered but not used and an explanation of why these models were not used. The description of the rejected alternative models does not need to be as detailed as the description of the models actually used in the CCA (and described under Section 194.23(a)(1)).

2.3 DOE METHODOLOGY AND CONCLUSIONS

2.3.1 Location of Information

DOE provides extensive discussion of the conceptual models used to describe the WIPP's performance in Chapter 2, Chapter 6.4 (pp. 6-78 to 6-214), and Chapter 9.3.1 (pp. 9-9 to 9-120). Additional information on alternative conceptual models was included in Appendix MASS. For example, Appendix MASS.2 (pp. MASS-2 to MASS-11) discusses the evolution of the WIPP conceptual models from the beginning of site selection in 1975. Also, Appendix MASS, Attachment 8-1, discusses the reasons why DOE discontinued work on the reaction path model for gas generation and chose to continue to use the average stoichiometry model for gas generation in the PA (see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Docket A-93-02, Item V-B-6, Section 2.0).

The Conceptual Models Peer Review Panel consideration of alternative conceptual models is described in Appendix PEER.1. Although the FEP screening analysis was not intentionally designed to assist the development of alternative conceptual models, DOE also used information generated during this process to support alternative conceptual model development (see Appendix MASS).

DOE did not include a detailed discussion of alternative conceptual models in the CCA. However, DOE subsequently provided a table with an explanation of alternative conceptual models in supplementary documentation submitted to EPA in a February 7, 1997, letter (Docket A-93-02, Item II-I-07); see Table 2 below. This table was prepared in response to an EPA letter dated December 19, 1996 (Docket A-93-02, Item II-I-01). As noted in Table 2 of this CARD, DOE listed alternative models it considered and explained why they were not used in the PA modeling calculations.

2.3.2 DOE Methodology

According to DOE, the original overall conceptual model remains valid today, although some of the details have changed since it was developed in the late 1980s. Principal elements of the model are listed below (Appendix MASS, pp. MASS-10 to MASS-11):

Repository Behavior

- ◆□ The waste horizon (the layer in which the waste is located in the repository) is not effectively isolated from nearby anhydrite interbeds.
- ◆□ Creep closure of salt beds in the Salado Formation occurs but does not ensure complete consolidation of the waste and surrounding rock.
- ◆□ The repository can become partially to fully saturated with liquid.

Gas Generation in the Repository

- ◆□ Gas is generated primarily by metal corrosion and microbial processes.
- ◆□ Gas generation is closely linked to other processes.
- ◆□ High gas pressures in the repository can induce fracturing of Salado interbeds.
- ◆□ High gas pressure (> 8 MPa) is necessary before spalling and direct brine releases can begin.

Transport through the Culebra

- ◆□ The Culebra dolomite is the most transmissive upper geologic unit, and releases through other overlying units are unlikely.
- ◆□ Transport of radionuclides through the Culebra dolomite is complex and sensitive to fractures and retardation.

Impacts of Human Intrusion

- ◆□ Borehole intersections with the repository and brine in the Castile layer are possible.
- ◆□ Brine inflow from the Salado is likely.
- ◆□ Multiple intrusions allow the possibility of flow between different boreholes.

Solubility

- ◆□ Actinide solubilities are important.

DOE's position is that the basic elements of the conceptual models used in the CCA have been developed over a number of years as a result of continuing analysis of alternatives and elimination of those alternative conceptual models found to be unacceptable or inappropriate. Some of this evolutionary history is included in Appendix MASS, but as noted in Section 2.3.1 above, a succinct presentation on alternatives was not provided in the CCA. Supplementary information provided by DOE in response to a request from EPA for information addressing the requirements of Section 194.23(a)(2) summarizes alternative models, as reviewed in Table 2 below.

2.4 EPA COMPLIANCE REVIEW

EPA reviewed the material on alternative conceptual models included in the CCA and the comments made by the Conceptual Models Peer Review Panel on alternative conceptual models. The Peer Review Panel identified no substantive issues regarding alternative models (Appendix PEER.1).

After its initial review of the CCA, EPA informed DOE that a complete discussion of alternative models that DOE seriously considered was required. In addition, EPA required additional information on DOE's treatment of transmissivity in the Culebra, as well as an alternate conceptualization treating the Culebra as an unconfined system (Docket A-93-02, Item II-I-01). In response, DOE provided a table with an explanation of alternative conceptual models in supplementary documentation submitted to EPA on February 7, 1997 (Docket A-93-02, Item II-I-07); see Table 2 below. DOE specifically addressed EPA's questions about Culebra transmissivity and treating the Culebra as an unconfined system in a sensitivity analysis (Docket A-93-02, Item II-I-16). EPA found that the sensitivity analysis results supported DOE's treatment of Culebra transmissivity and treatment of the Culebra as an unconfined system because of the minimal impact that changing assumptions had on results.

DOE stated that there were no obvious alternatives to some of the models used in PA (Docket A-93-02, Item II-I-07). DOE's summary of alternative conceptual models that were seriously considered but not used in PA is included in Table 2. The last column in the table indicates the section of the Conceptual Models Peer Review Panel Report (CCA Appendix PEER.1) that discusses alternatives to the selected models. In several instances the selected conceptual model was a modeling simplification rather than a true alternative model. For example, two-dimensional rather than three-dimensional geometry might be used in the computer codes.

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
Section 6.4.2.1 - Disposal System Geometry			
The system is represented by a two-dimensional vertical plane for BRAGFLO modeling and by assuring that flow is both convergent and divergent away from the repository. <i>This is a modeling simplification issue.</i>	Use of a three-dimensional model.	Appendix MASS, Attachment 4-1, explains why a three-dimensional model does not give significantly different result. Therefore, the two-dimensional model is used for computational efficiency.	3.1 3.3
The Salado is represented by impure halite with marker beds MB138 and MB139 and anhydrite layers a and b (lumped together) also modeled explicitly. <i>This is a modeling simplification issue.</i>	Use of a more detailed representation of Salado stratigraphy.	Section 6.4.5.1 refers to Christian-Frear and Webb (1996), which shows that a more detailed representation does not significantly change the PA results; therefore, the simpler model was used for the CCA calculations.	3.1
Section 6.4.2.2 - Culebra Geometry			
Flow in the Culebra can be represented by a numerical flow model which is supported by an extensive hydrologic data base.	Variability of Culebra hydrogeological properties is controlled by halite dissolution, topographic load, and other site characteristics.	The peer review panel concluded that the selected model meets the needs of the PA.	3.2
The Culebra is represented by a two-dimensional horizontal geometry for SECO modeling. <i>This is a modeling simplification issue.</i>	Use of a three-dimensional model.	Appendix MASS, Attachment 15-7 describes how a three-dimensional ground water basin model has been used to show that the two-dimensional model used in the disposal system calculations is adequate and no alternative treatment is necessary.	

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA (continued)

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
Section 6.4.3.1 - Creep Disposal			
Creep disposal in the vicinity of the excavation is modeled by calculating a porosity surface based on creep disposal and waste consolidation and linking it to gas generation and brine inflow. Creep is modeled using flow laws that fit available, relevant data.	An empirical reduced-modulus (RM) model was devised by Sjaardema and Drieg (1987). Several alternative flow laws exist.	Section 6.4.3.1 refers to Freeze et al. (1995), and Appendix PORSURF, Section 1 refers to Freeze (1996), which concludes that the selected model approximation is adequate. Appendix PORSURF, Attachments 1 and 7 discusses the model.	3.19
The porosity and permeability of the operational and experimental regions are fixed. <i>This is a modeling simplification issue.</i>	Use of porosities reflecting changes over time.	Appendix MASS, Section 7.1 and Appendix PORSURF, Section 4 and reference to Vaughn et al. (1995) show that the alternative treatment does not generate significantly different results. Therefore a simplified model was opted for.	3.3
Creep disposal is modeled using a 2-D representation of a single room. <i>This is a modeling simplification issue.</i>	Model multiple panels and their disposal.	Appendix PORSURF, Attachment 1 justifies the simplified treatment and refers to Osnes and Labreche (1995).	
Section 6.4.3.2 - Repository Flow			
Flow into the repository from the far-field is through naturally-occurring pore spaces in response to potentiometric gradients.	Assume the interconnecting pore space is only of limited extent and is due to excavation of the repository.	These alternatives are described in Appendix MASS, Section 7 and references therein. The far-field flow model was selected because its results cover those of the other two, and because of uncertainty as to the most realistic model.	3.5

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA (continued)

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
	Assume that the most significant source of brine inflow is through the clay layers exposed during excavation, and that flow through other lithologies within the Salado is negligible by comparison.		
The Brooks-Corey equation is used to represent interaction between brine and gas.	Use the Van Genuchten/Parker equation.	Both models are included in BRAGFLO, as described in Appendix BRAGFLO, Section 4.9. Appendix PEER, Section 1, p. 3-20 (the Peer review report) refers to Christian-Frear and Webb (1996) to justify the use of the Brooks-Corey treatment.	
All liquids in the repository have the same physical properties as Salado brine	Assume that there are several other sources of liquid in the repository such as the waste, operational activities, and Castile brine in the event of a borehole intrusion. Model the different liquids with their different flow properties. <i>This is a modeling simplification issue.</i>	The significance of these alternative fluid sources in terms of physical properties is discussed in Appendix MASS, Section 3.3, where it is shown to be of low significance. The model adopted is simpler.	

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA (continued)

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
Section 6.4.3.3 - Gas Generation			
Gas Generation was calculated using an average stoichiometry model based on metal corrosion and organic biodegradation on brine availability.	Assume passivation of steel by microbial-produced gas, and reduce gas generation from corrosion processes (the reaction path model).	Appendix MASS, Sections 8 and 8.1 describe the average stoichiometry model and its historical development. An alternative mathematical representation of this model not accounting for the relationship to brine availability was considered in earlier PAs. Appendix MASS, Attachment 8-1 and Attachment 8-3 document the reaction path model and why the average stoichiometry model was selected.	3.2.1
Section 6.4.3.4 - Chemical Conditions in the Repository			
Chemical conditions in the repository are constant and, with the exception of redox and gas generation reactions, at equilibrium with the backfill.	Assume that chemical equilibrium is not achieved with the backfill either immediately or over time as the backfill is consumed.	Chapter 9, Sections 9.3.1.2.10.2 and 9.3.2.2.2.2 discuss the likelihood of the backfill fulfilling its buffering role over a 10,000 year period.	3.22
Four undisturbed performance and E2 scenarios, the brine composition in the repository is that of Salado brine. For E1 scenarios, the composition is that of Castile brine.	Assume that in E1 scenarios, the brine composition will be a mixture between Salado and Castile brine, and that the solubility is determined by the mixture proportions. <i>This is a modeling simplification issue.</i>	The alternative is discussed in Appendix SOTERM, Sections 2.2.1 and 7.2.1. The alternative would introduce further uncertainty into the modeling. The effects on solubility are encompassed by the selected model.	

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA (continued)

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
<p>A condition of redox disequilibrium will exist between the possible oxidation states of the actinides.</p>	<p>Assume the actinides will be in redox equilibrium with the conditions in the repository.</p>	<p>Appendix SOTERM, Section 2.2.3 discusses the alternatives of oxidizing conditions in the repository and redox equilibrium. Appendix SOTERM, Section 4 discusses the likely oxidation states based on experimental observation and why the alternative states are not considered.</p>	
<p>Section 6.4.3.5 - Dissolved Actinide Source Term</p>			
<p>The solubility of different actinides can be calculated using an equilibrium thermodynamic model employing Pitzer interaction coefficients and assuming that, for a given oxidation state, the actinides exhibit similar chemical behavior and thus have the same solubilities.</p>	<p>Assume that each actinide has a significantly different chemical behavior and solubility for each of its oxidation states, and solubility can only be determined using a complete thermodynamic database.</p> <p>Assume that the system is not at or cannot be properly modeled at thermodynamic equilibrium, and that a conservative approach is to use inventory limits with maximum concentrations.</p>	<p>Appendix SOTERM, Section 3 dismisses the alternative of deriving a full thermodynamic database through experimental measurements as not logistically feasible. The inventory-limited model is too conservative and unrealistic. The adopted model considers the best constrained parts of the system (i.e., conservatively ignores sorptions, co-precipitation, etc.). The approach is justified by comparison to the available experimental data in Appendix SOTERM, section 3.6. The Pitzer formulism is justified compared to alternatives such as SIT.</p>	<p>3.23</p>

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA (continued)

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
Section 6.4.3.6 - Colloid Actinide Source Term			
Colloids present in the disposal room will consist of mineral fragments, intrinsic colloids, microbes and humic acids. Actinide concentrations associated with intrinsic colloids and mineral fragments can be treated as inventory-limited constants based on experimental detection limits. Humic and microbe colloid actinide concentrations can be modeled as thermodynamically-related to dissolved actinide concentrations, with a constant maximum concentration.	A full chemical equilibrium model where concentrations of actinides associated with all colloids are calculated based on equilibrium thermodynamics (and possibly accounting for sorption).	The adopted conceptual model is a mixture of the two alternatives. Appendix SOTERM, Section 6 and Appendix WCA, Attachments 18-5 to 18-8, document the selection of the model and the derivation of parameter values from experimental observation. The full chemical equilibrium alternative is too complicated and too uncertain to model. The inventory-limited alternative is conservative, but less realistic.	3.24
	An inventory-limited model with realistic maximum concentrations set by experimental observation.		
Section 6.4.4 - The Shaft System			
The four shafts connecting the repository to the surface are represented in BRAGFLO by a single shaft with a cross-section and volume equal to the total volume of the four real shafts and separated from the waste by the distance of the nearest real shaft.	A more realistic system with all four shafts represented individually. <i>This is a modeling simplification issue.</i>	Appendix MASS, Section 12.1 documents the development of the conceptual model. It refers to the 1992 WIPP PA, which considered alternative model representations. The peer review report, Section 3.1, pp. 3-3 and 3-4 discusses the alternative approach given here, but accepts the conservative nature of the model used. Otherwise, the representation of the seal in the PA is based on the seal design, and there are no alternatives.	3.1

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA (continued)

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
The shaft is surrounded by a DRZ which heals with time. The DRZ is represented through the permeabilities of the shaft system itself, rather than as a discrete zone. <i>This is a modeling simplification issue.</i>	Model the DRZ around the shafts as a discrete zone with permeability changing over time.	The DRZ model basis is described in Appendix SEAL, Section 7.5 and Appendix D.5. Representation of the DRZ through shaft permeabilities is justified in Appendix IRES.2, as referenced in Section 6.4.4.	
Section 6.4.5 - The Salado			
Interbeds have a fracture-initiation pressure above which local radial 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.	Assume anisotropic fracturing, preferential fracture orientations determined by dip and pre-existing fractures, and different fracture propagation laws.	Appendix MASS, Attachment 13-2 dismisses the alternative as unlikely.	3.6
The permeability of the DRZ around the repository is constant and higher than intact Salado. <i>This is a modeling simplification issue.</i>	Decrease the permeability with time and salt creep to that of Salado halite.	Appendix MASS, Section 13.4 refers to Vaughn et al. (1995), who showed that the alternative did not significantly affect results.	3.7
Section 6.4.6 - Units above the Salado			
Above the Salado, lateral actinide transport to the accessible environment can occur only through the Culebra. <i>This is a modeling simplification issue.</i>	Model transport through the Magenta and/or the Dewey Lake formations.	The alternatives are dismissed in Chapter 6.4.6.4 and 6.4.6.6, and the argument is expanded in Chapter 9.3.1.2.4. Appendix MASS, Section 14.1 refers to Barr et al. (1983) for modeling of the Magenta, and Beauheim (1986) for permeability measurement of the Dewey Lake. See also Wallace et al (1995), as referred to in Chapter 6.4.6.6.	

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA (continued)

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
Section 6.4.6.2 - The Culebra			
For fluid flow, the Culebra is modeled as a uniform (single-porosity) porous medium with spatially variable transmissivity.	Use a dual-porosity model.	The single porosity model simplification is justified in MASS Attachment 15-7 and Section 6.4.6.2 (p. 6-129).	3.2
	Use a discrete-fracture model.		
Recharge to the two-dimensional model of the Culebra is treated using constant head conditions on the regional grid boundaries. No vertical flow is modeled.	Include vertical recharge and leakage terms in the two-dimensional model. <i>This is a modeling simplification issue.</i>	The treatment of vertical flow is justified in Appendix MASS, Section 14.2, Appendix MASS Attachment 15-7 (p. 21), and Corbet and Knupp (1996), as referenced in Section 6.4.6.	
Section 6.4.6.2.1 - Transport of Dissolved Actinides in the Culebra			
Radio nuclide transport is modeled using a double-porosity model with the advective porosity representing fracture flow and the diffusive porosity representing matrix flow.	Use a single-porosity model.	Appendix MASS, Section 15.1 and Attachment 15-6 justifies the selection of the PA model.	3.10
	Use a discrete-fracture model.		
Sorption is modeled using a linear isotherm.	Use other models such as the Langmuir and Freundlich isotherms.	Appendix NUTS, Section 4.3.6 discusses the alternative models.	

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA (continued)

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
Section 6.4.6.2.2 - Colloid Transport in the Culebra			
Humic colloids are modeled as dissolved species. <i>This is a modeling simplification issue.</i>	Assume that humic substances influence the sorption behavior of dissolved actinides.	Appendix MASS, Section 15.3.1 describes results of experimental studies that show that the presence of humic substances in brine does not influence the sorption behavior of dissolved actinides.	
Actinide-bearing microbial and mineral colloids in the repository are filtered out and are not transported in the Culebra. <i>This is a modeling simplification issue.</i>	Use SECOTP2D (and underlying modeling assumptions) to model the effects of colloid retardation and transport phenomena.	Appendix MASS, Sections 15.3.1 and 15.3.3 describe results of experimental studies that show that colloidal actinides are strongly attenuated or present in negligible concentrations in the Culebra.	
Section 6.4.7.1 - Release During Drilling			
Direct brine release through a borehole will have negligible long-term effect on repository pressure and saturation. <i>This is a modeling simplification issue.</i>	Assume that direct brine release through a borehole affects the repository pressure and saturation.	Chapter 6.4.7.1.1 states that the effects are transient and local and are not significant to PA results.	
Activities of each drum in a stack of three which may be intersected by a borehole are independently sampled from 569 different waste streams.	Drum activities in a 3-stack are all from the same waste stream.	Section 3.13 of the Conceptual Models Peer Review Panel's Supplementary Report (Docket A-93-02, Item II-G-12) concludes that the selected model is adequate.	
Entrainment of brine and waste from a waste panel results from single-phase gas flow (spallings) and brine flow (direct brine release).	Assume that two-phase liquid/gas releases during inadvertent intrusion will entrain brine and waste solids.	Section 3.15 of the Conceptual Models Peer Review Panel's Supplementary Report (Docket A-93-02, Item II-G-12) concludes that the selected model is adequate.	

Table 2
DOE's Table Showing Alternative Conceptual Models Seriously Considered in the CCA (continued)

Model	Alternative Model	Discussion	Appendix PEER.1 Section (where applicable)
Fractures in the DRZ around the walls will heal during the period of active and passive institutional controls. Drilling into this region will not lead to direct brine releases.	Open fractures within the DRZ increase local halite permeability and allow migration of brine and gas to a borehole drilled in this region.	Section 3.15 of the Conceptual Models Peer Review Panel's Supplementary Report (Docket A-93-02, Item II-G-12) concludes that the selected model is adequate.	
Section 6.4.7.2 - Long-Term Releases Following Drilling			
The panels are not interconnected for long-term brine flow. <i>This is a modeling simplification issue.</i>	Assume that the panels are interconnected for long-term brine flow.	Chapter 6.4.13.6 states that this is a reasonable simplification based on detailed BRAGFLO calculations.	
Section 6.4.8 - Castile Brine Reservoirs			
Castile brine reservoirs have limited extent and interconnectivity, with effective radii on the order of several hundred meters.	Assume that Castile brine reservoirs have effective radii much larger than the waste panel dimensions.	Chapter 6.4.8 describes how it is conservative to assume reservoirs are of limited extent and are thus not depleted by multiple drilling penetrations in the vicinity of the WIPP. Reservoir volumes are described in Appendix MASS, Attachments 18-3 and 18-5.	3.16

Additional EPA comments on alternatives to the various conceptual models are included in Section 2.0 of EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6). EPA found that the supplementary information adequately described alternative models considered but not used because DOE sufficiently documented its rationale and approach to selecting the conceptual models used in the PA.

One of the models of particular concern to both EPA and the Conceptual Models Peer Review Panel was the spallings model. This model addressed blowout of waste particles from the repository during a drilling intrusion if the repository is pressurized above 8 megapascals (MPa) by gas generation and inward creep closure of the Salado halite. Pressures that are lower than 8 MPa are insufficient to overcome the hydrostatic head (or downward pressure) exerted by the drilling fluid and therefore cannot exert enough pressure to blow the waste particles to the surface. Because the spallings model used in the CCA was judged to be inadequate by the Conceptual Models Peer Review Panel, DOE developed a new mechanistically based computational approach to estimate the volume of spallings released to the land surface. The spallings model used in the CCA simulated only the end state of the spallings process. In contrast, the mechanistically based approach simulates the complete response of the system to the intrusion event from the time the repository is penetrated until the spallings event is terminated by reduction of tensile stresses on the waste. In the new mechanistically based model, several computational approaches were used to assess the magnitude of the spallings release, and quantitative agreement was obtained among the various approaches, thus adding credibility to simulation procedures. The volumes of released material calculated by the mechanistically based model were well below those predicted in the CCA. Even when the gas pressures were near lithostatic, the calculated spallings releases from the mechanistic model were lower than those estimated in the PA spallings calculations (Docket A-93-02, Items II-G-22 and II-G-23). Since it was demonstrated that the model used in the PA predicted conservative results, use of the original model's results (though not the model itself) was accepted by the Conceptual Models Peer Review Panel.

EPA later required DOE to perform additional PA calculations in a PAVT in order to verify that the cumulative impact of all potential problems in codes, parameters, and assumptions incorporated in the PA would not compromise the WIPP's compliance with the containment requirements of Section 191.13. In the PAVT, spallings volumes were sampled uniformly over a range from 0.5 to 4 m³ for all realizations in which the repository pressure exceeded 8 Mpa, rather than using a spallings model (Docket A-93-02, Item II-G-26, PAVT, p. 5-1). This range resulted from the PA spallings calculations (see Docket A-93-02, Item II-G-07, p. 4-12). This modeling approach was judged by EPA to be reasonable, given the determination that the spallings model in the CCA, though inadequate, nevertheless overestimated releases (Docket A-93-02, Item II-G-22, Section 4.0).

During the public comment period on EPA's proposed certification decision, the Agency received several comments suggesting a need for alternative conceptual models. EPA received comments on DOE and EPA's treatment of spallings and other analyses and DOE's decision to model only the "blowout" spallings mechanism and not "stuck pipe" or "gas erosion" mechanisms. The public also commented that certain aspects of WIPP geology should be modeled differently. In particular, commenters expressed concern that DOE's simplified

geometry for the repository in two dimensions might underestimate brine inflow and direct brine releases, compared to a three dimensional model geometry. Commenters stated that DOE's BRAGFLO code did not properly model anhydrite fracturing in anhydrite markerbeds in the Salado. They stated that DOE should use a model based upon linear elastic fracture mechanics.

For a general discussion of these issues and EPA's responses, see the "Modeling and Performance Assessment" section of the preamble. For a detailed discussion of these issues, see the following sections in the Response to Comments, Section 5: General Spallings Comments, SNL/DOE's Spallings GASOUT Computer Code, Stuck Pipe, Gas Erosion, and Related Waste Permeability, 2D vs. 3D BRAGFLO Modeling, Anhydrite Fracturing, and Anhydrite Interbed comments.

3.0 REQUIREMENT

(a) "Any compliance application shall include:

(3) Documentation that:

(i) Conceptual models and scenarios reasonably represent possible future states of the disposal system."

3.1 ABSTRACT

DOE convened a Conceptual Models Peer Review Panel to review the 24 conceptual models used in the PA. Among the issues considered by the peer review panel was whether conceptual models reasonably represented possible future states of the disposal system. See Section 7.0 of this CARD for a discussion of the conclusions of the Conceptual Models Peer Review Panel and EPA's review.

4.0 REQUIREMENT

(a) "Any compliance application shall include:

(3) Documentation that:

(ii) Mathematical models incorporate equations and boundary conditions which reasonably represent the mathematical formulation of the conceptual models."

4.1 ABSTRACT

EPA performed an independent review of the computer codes used to support the PA. This review focused on whether mathematical models incorporated equations and boundary conditions that reasonably represent the mathematical formulation of the conceptual models reviewed under Section 194.23 (a)(1). EPA reviewed information contained primarily in User's Manuals, Validation Documents, Implementation Documents, and Requirements Document &

Verification and Validation Plans for each PA computer code (see Docket A-93-02, Item II-G-3). EPA reviewed the mathematical model equations and boundary conditions for the following codes: CUTTINGS_S, SECOFL2D, SECOTP2D, CCDFGF, PANEL, BRAGFLO, BRAGFLO_DBR, NUTS, FMT, SANTOS and GRASP-INV. 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 Section 4 of EPA Technical Support Document for Section 194.23: Models and Computer, Docket A-93-02, Item V-B-6, for a detailed discussion of these problems). As discussed below, DOE satisfactorily resolved all of the difficulties related to the equations that make up the mathematical models and the incorporation of the boundary conditions of the various codes.

4.2 COMPLIANCE REVIEW CRITERIA

The CCA should provide a thorough discussion of the development of mathematical model equations based on the conceptual models. The primary objective of EPA's review for this subsection was to determine whether:

- ◆ DOE provided an adequate technical basis to support the mathematical formulations developed from the conceptual models and scenarios selected for modeling and then used in the PA.
- ◆ DOE provided adequate descriptions and explanations of those mathematical formulations.
- ◆ Boundary conditions of conceptual models were reasonable representations of how the models should be used. In several instances, DOE's mathematical models incorporated equations that describe simplified conceptual models (e.g., distribution coefficients for sorption) that may lead to approximate solutions.

4.3 DOE METHODOLOGY AND CONCLUSIONS

4.3.1 Location of Information in the CCA

Information regarding computer codes mathematical model equations and boundary conditions is contained in documents that were developed for each of the PA computer codes. These documents are available from the Sandia National Laboratory (SNL) record center and are described below. See Docket A-93-02, Item II-G-3, Volumes 1-12, for a list of each computer code's specific documents. See EPA Technical Support Document for Section 194.23: Models and Computer Codes, Appendix A (Docket A-93-02, Item V-B-6) for a discussion of each computer code. See Section 6.0 below for further discussion of these documents.

- ◆ User's Manual—describes each code's purpose and function, instructions on use of the code, and the models and methods employed by the code. Examples of user input and output files are typically included.

- ◆ □ Validation Document—for individual codes, summarizes the results of the testing activities prescribed in the Requirements Document & Verification and Validation Plan (RD/VVP) discussed below, and provides evaluations of how well the code matches other known solutions based on those results.
- ◆ □ Implementation Document—provides the information necessary for the recreation of the code as used in the 1996 WIPP PA calculation. With this information the user can compile the code or can install it on a platform identical to that used in the 1996 WIPP PA calculations. The document includes the source-code listing, the subroutine call hierarchy, and information required to compile executable versions of the code.
- ◆ □ Requirements Document & Verification and Validation Plan—identifies the computational requirements of the code and describes how the code will be tested to ensure that those requirements are satisfied.

A unique set of these four documents exists for each PA computer code, with the exception of SANTOS. These four documents for SANTOS are included in the SANTOS Quality Assurance Document (QAD) and the Verification and Qualification Document (V&QD); see Volume 11 of Docket A-93-02, Item II-G-3).

4.3.2 Mathematical Model Equations

Five computer codes are used to solve mathematical model equations that incorporate a mathematical formulation of conceptual models of the future characteristics of the waste repository: SANTOS, BRAGFLO, FMT, NUTS, and PANEL. The SANTOS computer code consists of mathematical model equations that predict the mechanical collapse of the repository through salt creep closure of the Salado. These equations are used to predict void space porosities based on the ambient pressure in the repository. This relationship of pressure versus porosity is then used in the BRAGFLO computer code to calculate the impact of Salado salt creep closure (Appendix BRAGFLO.4.11). The primary mathematical model equations that comprise BRAGFLO predict gas generation rates, brine and gas flow, and fracturing within the anhydrite marker beds in order to calculate future conditions of the repository (Appendix BRAGFLO.4). In addition to these mathematical models equations, BRAGFLO_DBR uses the BRAGFLO formulation, with the addition of the mathematical treatment of a well drilled into the waste, to calculate the amount of waste dissolution in brine and transport of the contaminated brine (Appendix BRAGFLO_DBR.4). The results of the BRAGFLO and BRAGFLO_DBR calculations are then used by the NUTS and PANEL computer codes (see below).

FMT is a computer code that consists of mathematical models equations that predict actinide solubilities based on thermodynamics assumptions (Appendix SOTERM, Attachment 1, Section 4). The actinide solubilities are used in NUTS and PANEL to calculate the actinide concentrations release from the repository.

NUTS and PANEL use outputs from BRAGFLO, BRAGFLO_DBR and FMT to calculate actinide concentrations released from the repository. NUTS is coupled with BRAGFLO and BRAGFLO_DBR via the ground water flow field, i.e., the volume of waste-contaminated brine that is calculated to leave the repository. BRAGFLO predicts the magnitude and directions of gas and brine velocities. NUTS uses mathematical model equations to scale the magnitude of the BRAGFLO releases using the actinide solubilities (Appendix NUTS.4). PANEL's mathematical model equations predict actinide solubilities as a function of oxidation state and radioactive decay and also predict actinide concentrations released (Appendix PANEL.4). BRAGFLO, NUTS, and PANEL mathematical model equations together describe radionuclide contaminant dissolution and precipitation, advective transport, and radioactive decay and predict the actinide concentrations released from the repository (Appendices NUTS, PANEL, and BRAGFLO.4).

Three computer codes are used to solve mathematical model equations that incorporate a mathematical formulation of conceptual models of flow and transport of waste-laden brine in the Culebra dolomite: GRASP-INV, SECOFL2D, and SECOTP2D. The mathematical model equations that comprise GRASP-INV are based on spatial correlations designed to predict the Culebra dolomite transmissivity fields that affect the rates at which radionuclides migrate through the Culebra dolomite (Appendix TFIELD, Section Tfield 3). The results of the GRASP-INV calculations are used as input to the SECOFL2D computer code. The primary mathematical model equations incorporated into SECOFL2D describe advective (rock matrix) ground water flow through the Culebra dolomite in two dimensions, using the releases predicted by the BRAGFLO, NUTS, and PANEL computer codes (Appendix SECOFL2D.3, pp. 10-19). SECOTP2D extends the mathematical model equations of SECOFL2D to calculate the transport of contaminated waste through the Culebra dolomite and to calculate radioactive decay, dispersion, and molecular diffusion (Appendix SECOTP2D.2).

One computer code, CUTTINGS_S, is used to solve mathematical model equations that incorporate a mathematical formulation of conceptual models for the removal of solid waste from the repository due to human intrusion drilling. The mathematical model equations that make up CUTTINGS_S predict the volume of waste released due to cavings² and drill cuttings³ that occur if a borehole penetrates the waste. The mathematical model equations in CUTTINGS_S also predict spallings releases⁴ if the upward pressure exceeds 8 MPa when the intrusion borehole penetrates the waste in the repository (Appendix CUTTINGS.4).

One computer code, CCDFGF, is used to solve mathematical model equations that incorporate a mathematical formulation of conceptual models of multiple combinations of future drilling events. The CCDFGF computer code uses mathematical methods that predict the

² "Cavings" refers to material that falls from the walls of a borehole as a drill bit penetrates.

³ "Cuttings" refers to material that is actually cut by a drill bit during drilling, including any waste that may be intersected in the repository.

⁴ "Spallings" refers to releases of solids pushed up and out of a borehole by gas pressure in the repository.

likelihood that brine reservoirs are intercepted (i.e., number of drill hits) and predict how fast a Castile brine pocket would be depleted in order to calculate the complementary, cumulative distribution functions (CCDFs) used to show compliance with EPA containment requirements (Appendix CCDFGF.2, pp. 3-6).

4.3.3 Boundary Conditions

The following codes used in DOE's PA require initial and boundary conditions: SANTOS, BRAGFLO, BRAGFLO_DBR, SECOFL2D, SECOTP2D. These codes use mathematical model equations that solve partial differential equations by considering rates of change; thus, these codes need initial and boundary conditions between which the rates of change in the equations will operate. The SANTOS computer code models Salado salt creep closure and provides the resultant porosity surface to the BRAGFLO computer code. The computer code NUTS is strongly coupled to the results of the BRAGFLO calculations in a manner analogous to the way in which the computer code SECOTP2D is coupled to the computer code SECOFL2D (Appendix CODELINK contains flowcharts that relate the PA computer codes).

The computer code NUTS calculates the transport of radionuclides based on the BRAGFLO computational grid system, which uses the fluid flow characteristics calculated by the computer code BRAGFLO. The computer code NUTS uses the pressure, flow rates, and initial conditions calculated in the BRAGFLO computer code. Boundary conditions for advective transport are consistent with the boundary conditions assumed for fluid flow. Actinide concentrations are initially zero in all regions except in the waste. Actinide concentrations in brine in the waste regions are assigned as discussed in Chapter 6.4.3.5 (pp. 6-107 to 6-109).

The computer code PANEL is used to estimate the transport of radionuclides from the repository to the Culebra for the E2E1 scenario only (i.e., interception of both the waste and a brine reservoir by a borehole); see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Appendix A-2 (Docket A-93-02, Item V-B-06). PANEL assumes homogeneous mixing within a panel of the waste disposal region to calculate the actinide concentration that will be introduced into the Culebra dolomite as a result of a borehole intrusion (Volume XI, Appendix PANEL.5). PANEL is coupled to the results calculated by the BRAGFLO computer code and is used as input to the SECOTP2D computer code. An actinide concentration in the brine moving up the borehole and out of the waste panel is calculated with the BRAGFLO computer code and is subsequently used as input to the PANEL computer code in order to determine the mixing volume in PANEL (i.e., higher mixing volumes lead to lower actinide concentrations). Radionuclides leaving the location for mixing in PANEL are assumed to arrive at the Culebra. The SECOTP2D computer code uses the contaminant concentration calculated in the PANEL computer code as source-term⁵ input and calculates the transport of actinides through the Culebra dolomite.

⁵ The "source-term" is the radiation from the radionuclides in the repository and the chemical products of those radionuclides as they interact with materials in the repository.

Models for solid release to the surface are also coupled to the BRAGFLO computer code calculations. The CUTTINGS_S computer code (cuttings, cavings, and spillings) uses the results calculated by the BRAGFLO computer code. CUTTINGS_S uses fluid pressure, fluid saturation, and other necessary quantities from the BRAGFLO calculations to predict the solid waste released.

The computer code BRAGFLO_DBR uses the results of the BRAGFLO computer code calculations to predict the direct brine release of radionuclides to the surface. It is assumed that, once waste-laden brine is entrained into drilling fluid, the waste-laden brine remains in the borehole until it reaches the surface (Chapter 6.4.7.1.1, pp. 6-152 to 6-156). In other words, there is no interaction between drilling fluid and the overlying rock formations between the repository and the surface. This is a conservative assumption that overestimates potential releases. In the direct brine release model, brine is not allowed to enter any of the units above the repository (e.g., the Culebra Formation) and flows directly to the surface, because the borehole is assumed to be lined with steel protective casing from the top of the Salado to the surface.

4.4 EPA COMPLIANCE REVIEW

EPA reviewed each of the mathematical models for the computer codes used in the PA to determine if the governing equations (e.g., flow and transport governing equations), process-related equation(s) (e.g., the anhydrite fracture model), and boundary conditions (e.g., no flow boundary assumptions) included in each mathematical model provided a reasonable representation of each conceptual model used in the PA. The User's Manual and Analysis Package for each code were the primary sources of information on the mathematical models employed in PA (see Docket A-93-02, II-G-3, Volumes 1-12, for each code and Items II-G-04 to II-G-11 for each analysis package). In general, mathematical formulations were adequately explained and were reasonable. DOE adequately documented and described simplifications of conceptual models in the CCA. DOE provided an adequate technical basis to support the mathematical formulations.

No major issues resulted from the review of the mathematical model equations and boundary conditions. However, EPA noted some concerns regarding the BRAGFLO computer code. For example, during an internal review, DOE discovered that the governing equations were incorrectly formulated for a compressible fluid; see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 4.4.1.1 (Docket A-93-02, Item V-B-06). EPA specified that the equations in the code be corrected and that the changes to the code be documented; see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 4.4.1.1 (Docket A-93-02, Item V-B-06). DOE made the specified corrections and documented them in the User's Manual for the respective codes (Docket A-93-02, Item II-G-3, Volume 2). EPA also required that DOE provide additional information on the Appendix CCDFGF Design Document, and on the incorporation of wicking into the BRAGFLO mathematical model (Docket A-93-02, Item II-I-01). DOE documented this information in the User's Manual for the respective codes (Docket A-93-02, Item II-G-3, Volume 2) and in subsequent correspondence with EPA (Docket A-93-02, Item II-I-31).

Under its authority under Section 194.23(d), EPA required DOE to perform additional PA calculations in a PAVT to demonstrate that the cumulative impact of all the required changes in codes, parameters, and assumptions incorporated in PA were not significant enough to require a new PA. The results of the PAVT required by EPA demonstrated that the combined effect of all the required changes did not significantly alter the predicted performance of the repository.

EPA also reviewed the functional tests described in the Validation Document for each computer code to ensure that DOE's tests of the computer code demonstrated that the code performed as specified in the Requirements Document (Docket A-93-02, Item II-G-3, Volumes 1-12, for each code). EPA tested each of the codes to verify that DOE adequately tested functional requirements listed for each computer code. This analysis and testing indicated that equations and boundary conditions were properly incorporated into the mathematical models and that boundary conditions were reasonable representations of how the conceptual models should be implemented (see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 4.0, Docket A-93-02, Item V-B-6).

5.0 REQUIREMENT

(a) "Any compliance application shall include:

(3) Documentation that:

(iii) Numerical models provide numerical schemes which enable the mathematical models to obtain stable solutions."

5.1 ABSTRACT

EPA performed an independent review of the numerical models used in the computer codes. This review focused on evaluating whether the numerical models provide numerical schemes that enable the mathematical models to obtain stable solutions. For example, numerical models might include numerical solution methods, such as the TVD solver used for SECOTP2D or the Newton-Raphson solver in BRAGFLO. The relevant information was contained in User's Manuals, Validation Documents, Implementation Documents and Requirements Document & Verification and Validation Plans (see Docket A-93-02, Item II-G-3, Volumes 1-12, for each code). The codes that used numerical solvers include: SANTOS, CUTTINGS_S, SECOFL2D, SECOTP2D, PANEL, BRAGFLO, BRAGFLO_DBR, NUTS, and GRASP-INV. EPA's review identified stability concerns related to the numerical solution algorithms of the mathematical models associated with the following codes: CUTTINGS_S, SECOFL2D, SECOTP2D, and NUTS. In the case of the NUTS and SECOTP2D codes, DOE made 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 more testing results that showed these problems had been corrected. All EPA concerns regarding code stability issues were satisfactorily resolved.

5.2 COMPLIANCE REVIEW CRITERIA

EPA expected the CCA to provide a complete and logical discussion of the numerical solution algorithms used to implement the mathematical models required for the PA. This documentation must demonstrate that the numerical solution algorithms provided stable solutions.

5.3 DOE METHODOLOGY AND CONCLUSIONS

Information used to evaluate the stability of numerical model numerical schemes was provided in the Analysis Packages that DOE prepared for each of the PA computer codes (see Docket A-93-02, Items II-G-04 to II-G-11, for each analysis package). In these packages, testing results were provided for problems that were very similar to the ones that the code(s) solved in PA calculations. Such testing was performed to evaluate the stability of the numerical schemes used to solve the mathematical model equations.

DOE's evaluation of numerical schemes for determining software stability of numerical models included an evaluation of the impact on previous analyses and any appropriate corrective action to the computer code and/or earlier analyses. Errors that qualified as a condition adverse to quality, such a computer code stability problems, were controlled and resolved as described in Chapter 5.3.17 (pp. 5-36 to 5-37).

DOE maintains a computational record of whether any of the codes experienced stability problems during the PA calculations. This record is documented in the output for each code and notes the convergence criteria, the number of numerical iterations required to reach convergence, and the mass balance. Convergence criteria are set within various subroutines in the computer codes, where appropriate, and the maximum number of iterations allowed to achieve the convergence criteria are also built into the codes. Although DOE did not specify strict requirements for the convergence criteria, if the criteria are too lenient the results will indicate a high mass balance error and potentially unstable solutions to the numerical model numerical schemes. The code generates messages if the mathematical solution algorithm does not converge within the user-specified criteria (see the User's Manual for each computer code, Docket A-93-02, Items II-G-1 and II-G-3). Problems are generally documented in the Analysis Packages (Docket A-93-02, Item II-G-3).

5.4 EPA COMPLIANCE REVIEW

EPA reviewed all relevant documentation on numerical models solution schemes, which was primarily contained in CCA appendices (e.g., NUTS, SECOFL2D), Analysis Packages, and supplementary information (e.g., User's Manuals, Validation Documents). For more specific references, see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 5.0 (Docket A-93-02, Item V-B-6). EPA also reviewed the QA documentation packages for each code for completeness and technical adequacy; see Docket A-93-02, Item II-G-3, Volumes 1-12, for each code and Items II-G-04 to II-G-11 for each analysis package).

In addition, EPA successfully executed DOE code verification tests, as described in the Verification Documents for each of the respective PA codes (see Docket A-93-02, Item II-G-3, Volumes 1-12, for each code). In a few cases, stability problems were suspected and EPA requested that DOE conduct additional testing (see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 5.0, Docket A-93-02, Item V-B-6, and Docket A-93-02, Item II-I-17). EPA noted that four computer codes appeared to have stability problems: BRAGFLO, NUTS, SECOFL2D and SECOTP2D (see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Sections 4.4, 4.6 and 4.11, Docket A-93-02, Item V-B-6). EPA identified numerous errors in the NUTS code and required that DOE correct the source code for the computer program (Docket A-93-02, Item II-I-01). DOE determined that stability problems in the NUTS code were related to the method of introducing solubility limits into the code. These problems were rectified through the use of an explicit scheme to ensure convergence at the solubility limits for the various radionuclides. This additional work was completed by DOE and the stability issues were satisfactorily resolved. Additional discussion is provided in Section 5.0, and especially section 5.4.4, of EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6).

6.0 REQUIREMENT

(a) “Any compliance application shall include:

(3) Documentation that:

(iv) Computer models accurately implement the numerical models; i.e., computer codes are free of coding errors and produce stable solutions.”

6.1 ABSTRACT

EPA performed an independent review of the PA computer codes used to support the PA. As part of this review, EPA executed the functional tests outlined in DOE’s Validation Documents for each code in order to verify that the computer codes accurately implement the numerical models, are free of coding errors, and produce stable solutions. The information that EPA reviewed was primarily contained in User’s Manuals, Validation Documents, Implementation Documents, and Requirements Document and Verification and Validation Plans for each computer code. The codes that were reviewed include: SANTOS, CUTTINGS_S, SECOFL2D, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO_DBR, FMT, NUTS, GRASP-INV and ALGEBRA. EPA identified issues that were related to coding errors for the following codes: SECOFL2D, SECOTP2D, and NUTS. These issues were satisfactorily resolved, as discussed in Section 6.4 of this CARD.

6.2 COMPLIANCE REVIEW CRITERIA

EPA expected that documentation in the CCA would demonstrate that the computer models (codes) developed from numerical models were accurate and free of coding errors and produced stable solutions.

6.3 DOE METHODOLOGY AND CONCLUSIONS

To ensure that DOE's computer codes accurately implement the numerical models and are free of coding errors, SNL adopted a number of Quality Assurance Procedures (QAPs) (see CCA Appendix QAPD, Section 6, for software QA requirements). The QAPs specify quality assurance requirements for each step of the software development process (see **CARD 22—Quality Assurance** for a discussion of EPA's review of DOE's QA program). This process involved four primary development phases: 1) requirements phase, 2) design phase, 3) implementation phase and 4) software verification and validation (Appendix QAPD, Section 6.5). The objective of each of these phases is discussed below.

The requirements phase consists of defining and documenting both the functional requirements that the software must meet and the verification and validation activities that must be performed in order to demonstrate that the computational requirements for the software are met. Two documents are produced during this phase, the Requirements Document (RD) and the Verification and Validation Plan (VVP). The RD contains the functional requirements that the proposed software must satisfy. Specific requirements relate to the aspects of the system that must be simulated with a particular computer code. For example, ground water flow through the Culebra is assumed to be steady through time. Therefore, SECOFL2D was required to demonstrate that the flow equation provided accurate solutions over time under steady-state conditions. The VVP identifies tests to be performed and associated acceptance criteria to ensure verification of each software development phase (i.e., the aspect of the code being tested matches known solutions) and validation of the entire software baseline of the first time the computer code is placed under QA control (i.e., all aspects of the code work together properly).

The design phase consists of developing and documenting the overall structure of the software and the reduction of the overall software structure into descriptions of how the code works. During this phase, the software structural design may necessitate modifying the RD and VVP. The Design Document (DD) provides the theoretical model, the mathematical model, and the major components of the software. Because most of the PA computer codes were already developed before the PA calculations, the DD was not needed. SNL used the RD to document what the PA computer did by listing the functional requirements of each computer code. SNL used the VVP to explain various tests needed to show that the computer code properly performed the functional requirements list in the RD.

The implementation phase consists of developing a source code using a programming language (i.e., FORTRAN) or other form suitable for compilation or translation into executable computer software. The design, as described in the Design Document, is used as the basis for the software development, and it may need to be modified to reflect changes identified in the

implementation phase. Two documents are produced during this phase, the Implementation Document and the User's Manual. The Implementation Document provides the source code listing and describes the process performed to generate executable software, and the User's Manual provides information that assists the user in the understanding and use of the code.

The validation phase consists of executing the functional test cases identified in the VVP to demonstrate that the developed software meets the requirements defined for it in the VVP. The tests demonstrate the capability of the software to produce valid results for problems encompassing the range of permitted usage as defined by the User's Manual. One document, the Validation Document (VD), is produced during this phase. The VD documents the test case input and output files and evaluates the results versus the acceptance criteria in the VVP.

DOE used these procedures and documents to show that the PA computer codes calculate numerical models properly, and that the computer codes were free of coding errors and produced stable results.

6.4 EPA COMPLIANCE REVIEW

EPA reviewed all of the relevant documentation pertaining to each of the major codes described above (i.e., DD, RD, VVP and VD) and supplementary information sent by DOE (Docket A-93-02, Items II-I-02 to II-I-38). EPA also independently tested all of the computer codes by executing the tests outlined in the VVP. EPA identified a number of deficiencies related to this requirement. EPA required DOE to submit the following: (1) information to evaluate the testing of SECOTP2D; (2) the relevant FORTRAN code and documentation that it has been tested; (3) information to verify that the grid geometry in BRAGFLO and NUTS calculates accurate and stable results; (4) a test that the SECOFL2D code implements the transition from a regional grid to a local grid; (5) evidence that SECOTP2D correctly addresses longitudinal and transverse dispersities in the Culebra; and (6) an analysis of flow in the repository representative of an intrusion scenario in which brine reaches the Culebra (Docket A-93-02, Item II-I-01). DOE provided this additional information in several documents (Docket A-93-02, Items II-I-16, II-G-03, and II-I-31).

In addition, EPA required DOE to submit the following: (1) a test of SECOTP2D with a heterogeneous transmissivity field; (2) an analysis of mass balance in SECOTP2D; (3) identification of all errors in computer codes discovered by DOE since the PA calculations were run; and (4) additional information on tests described in Record 25, WPO 43367 (Docket A-93-02, Item II-I-17). DOE responded to these requests for additional information in a letter with the requested mass balance and test of SECOTP2D with a heterogeneous transmissivity field and SECOTP3D Code Test Results described in Record 25, WPO 43367 (Docket A-93-02, Item II-I-31). EPA also requested that DOE perform a quantitative impact analysis on code errors to determine whether the coding errors would have affected the CCA results. Results from the impact analysis indicate that the coding errors would have had very little impact on the WIPP's compliance with the disposal regulations (Docket A-93-02, Item II-I-31).

7.0 REQUIREMENT

(a) “Any compliance application shall include:

(3) Documentation that:

(v) Conceptual models have undergone peer review according to § 194.27.”

7.1 ABSTRACT

DOE convened a Conceptual Models Peer Review Panel to review the 24 conceptual models used in the PA (see Table 1 of this CARD). During the initial review, the Panel found that 13 models were adequate for use in the PA and 11 were not. Based on additional information provided by DOE, and three subsequent review sessions, the Panel found all models except the spallings model to be adequate for use in the PA. Based on additional analytical and experimental work provided by DOE (Docket A-93-02, Item II-G-23), the Panel ultimately found that the supplementary information was sufficiently accurate and complete to support the conclusion that the spallings values used in the CCA were reasonable for use in the PA, and in fact overestimate the actual waste volumes that would be expected to be released by the spallings process (Docket A-93-02, Item II-G-22). EPA concurs with the Panel’s findings.

7.2 COMPLIANCE REVIEW CRITERIA

The fundamental question that the peer review panel was expected to answer was, “Do the final conceptual models and the subsystem components used in the CCA represent a reasonable approximation of the actual disposal system?” The CCA must demonstrate that this question was fully addressed by a peer review performed and documented in accordance with the requirements of Section 194.27. The Peer Review Panel must have all relevant information on hand to ensure that decisions are sufficiently objective.

The CCA must document that the peer review was conducted in a manner consistent with NUREG-1297, which provides guidance for the proper conduct of a peer review related to high-level radioactive waste repositories. Such documentation must include:

- ◆ A list of the reviewers.
- ◆ Acceptability requirements for each reviewer.
- ◆ Individual statements by peer reviewers reflecting dissenting views.
- ◆ A discussion of the conceptual models peer reviewed.
- ◆ An evaluation of data and information used to develop conceptual models, including attributes of the disposal system learned during site

characterization activities, such as room creep closure or DRZ characteristics.

- ◆□ An evaluation of the validity of conceptual model assumptions.
- ◆□ An evaluation of alternate conceptual models.
- ◆□ An evaluation of the uncertainty in the conceptual models and a discussion of consequences if the conceptual model chosen is inappropriate for the site.
- ◆□ A statement indicating the adequacy of the conceptual models used for the disposal system.
- ◆□ A statement of the accuracy of the results based on the conceptual models employed.
- ◆□ A discussion of the validity of the conclusions drawn based on the conceptual models.

The first three of these items are discussed under **CARD 27—Peer Review**; all others are discussed below.

7.3 DOE METHODOLOGY AND CONCLUSIONS

The first round of activity of the Conceptual Models Peer Review Panel is described in detail in CCA Appendix PEER.1. This Appendix includes:

- ◆ The Conceptual Models Peer Review Plan prepared by the DOE Carlsbad Area Office.
- ◆ The Final Conceptual Models Peer Review Report prepared by the Conceptual Models Peer Review Panel, dated July 1996 (Appendix A to the report contains determinations of the independence of each peer review panel member and a certification regarding organizational conflicts of interests).

The Panel initially found 13 of the 24 conceptual models to be adequate for use in PA. After the CCA was issued in October 1996, the Conceptual Models Peer Review Panel met again to consider the remaining 11 models in light of additional information and responses provided by DOE. The Panel issued its first supplementary report in December 1996 (Docket A-93-02, Item II-G-12). Based on supplementary information, the Panel determined that nine additional conceptual models were adequate for use in the PA. Two conceptual models, Spallings and Chemical Conditions, were still deemed inadequate. DOE reconvened the Panel for a second time in January 1997; the results of these deliberations are included in a second supplementary report

(Docket A-93-02, Item II-G-21). The Panel once again rejected the Spallings and Chemical Conditions Conceptual Models. DOE reconvened the Panel for the last time in April 1997 to review new information on these models developed by DOE after January 1997 (Docket A-93-02, Item II-G-22).

DOE provided the Panel with a list of 24 conceptual models used in the PA (see Table 1 above). The Panel acquired the information necessary to review these models by (Appendix PEER.1, p. 2-10):

- ◆□ Reviewing literature related to the content and development of the conceptual models.
- ◆□ Attending briefings on conceptual models and relevant aspects of the PA process.
- ◆□ Conducting conceptual model or issue-focused presentations and question-and-answer sessions with DOE scientists and engineers.
- ◆□ Reviewing materials obtained through independent research and question-and-answer sessions.
- ◆□ Conducting formal and informal discussions among Panel members.
- ◆□ Touring WIPP facilities and the local area outside the WIPP site.

In its initial report, the Panel evaluated only information available to them as of June 7, 1996. In several instances, the conceptual models were undergoing development or revision at the time of the Panel's review. Consequently, final conceptual models were not always available for the Panel's review. Additionally, the final PA modeling used in the CCA had not been completed, so the panel initially had no knowledge of the end product resulting from the application of the conceptual models.

The Panel used nine criteria to decide on the adequacy of each of the 24 conceptual models (Chapter 9, pp. 9-4 and 9-11):

- ◆ Information used to develop the conceptual model.
- ◆ Validity of model assumptions.
- ◆ Evaluation of alternatives.
- ◆ Uncertainties.
- ◆ Adequacy of the conceptual model (including conclusions about whether the models reasonably represent future states of the disposal system).

- ◆□ Adequacy of application (i.e., whether the application of the conceptual model is appropriate for the CCA).
- ◆□ Accuracy of results (with respect to CCA).
- ◆□ Validity of conclusions.
- ◆□ Adequacy of implementation.

The “adequacy of implementation” criterion is a summary criterion that embraces judgments based on the other eight criteria. As stated by the Panel, adequacy of implementation is “an overall, bottom-line assessment of whether the conceptual models, as intended for use in the compliance application, represent a reasonable approximation of the actual disposal system based on the eight previous criteria” (Appendix PEER.1, p. 2-14).

Based on its initial evaluation, the Panel found that 11 of the models were inadequate but that two of the inadequate models were of no consequence to the PA. The Panel also initially deemed 13 of the 24 conceptual models adequate for use in the PA (Chapter 9.3.1.1, Adequate Models).

The Panel found 11 of the conceptual models to be inadequate for a variety of reasons (see Chapter 9.3.1.2, p. 9-16). Some models were deemed inadequate because it appeared that certain possibilities had not been considered in the development of the model, such as consideration of the potential for release or changes in repository conditions from borehole penetrations in the exploration boreholes conceptual model (p. 9-38). In other cases, the Panel found that the conceptual models did not incorporate some important physical conditions, such as the omission of how the bounding clay seams in the Salado interbeds might affect fracture propagation and permeability (p. 9-25).

For some conceptual models, the Panel found that the associated experimental data were not fully defensible, such as the distribution coefficient values (K_d s) for the transport of colloidal actinides in the Culebra (Chapter 9, p. 9-35). The Panel suggested that DOE should have performed a sensitivity analysis for some conceptual models. For example, the Panel recommended evaluation of the sensitivity of the PA for the reference conditions in a revised version of the model BRAGFLO, as part of the conceptual model for exploration boreholes (p. 9-53). Finally, in many cases the Panel believed that DOE had provided insufficient support for assumptions in the conceptual models, such as the expected probability of encountering pressurized brine below the repository in the conceptual model for the Castile and brine reservoir (*ibid.*, p. 9-71). For further information, see Appendix PEER.1, Section 5.0).

When the Panel reconvened in November 1996, they reviewed their earlier conclusions and found that all but two of the models were judged to be adequate based on additional information and analyses provided by DOE (Docket A-93-02, Item II-G-12). The two conceptual models that remained inadequate were Spallings and Chemical Conditions. The Panel found the

Chemical Conditions conceptual model to be inadequate because (Docket A-93-02, Item II-G-12, p. 70):

The ability of the magnesium oxide (MgO) backfill to react completely and rapidly with CO₂ to buffer the chemical system and limit actinide solubilities was not adequately substantiated by experimental physical results that correctly simulate conditions in the repository. Although the pH buffering assumptions are of considerable importance to many other conceptual models, the conclusion that the MgO will in fact perform as assumed was not adequately supported.

The Panel found the Spallings conceptual model to be inadequate because (Docket A-93-02, Item II-G-12, p. 70):

An adequate basis for the parameters used in the mathematical expression of the model was not developed. In particular, ignoring capillary forces and correlating tensile strength with surface erosion was not adequately supported by either first principles or experiment.

The principal assumptions upon which the mathematical model is based appear to be incomplete. Waste removal by entrainment in gas flow is expected to occur in a highly dynamic sequence principally involving a spalling process driven by gas flow out of the porous waste normal (perpendicular) to the eroded surface. The primary effect controlling the volume of spall is the subsequent erosion by gas flow parallel to the eroded surface in pathways that are not expected, particularly early after the WIPP ceases operations. In addition, DOE has not adequately shown that the steady-state assumption of the model conservatively approximates releases associated with the dynamic process of spall, and the possibility of transonic velocities has apparently not been considered.

The experiments conducted in support of this model appear to have been designed to reproduce the assumptions upon which the model is based, rather than to simulate the dynamic repository system. Although the experiments may support adoption of specific model parameters, they do not demonstrate that the model adequately represents future states of the repository (see Docket A-93-02, Item II-G-12, p. 74).

In addition, six of the models “were found to be adequate on the basis that no consequence to PA is anticipated.” The Conceptual Models Peer Review Panel’s position on questionable conceptual models as of December 1996 is summarized below:

<u>Model</u>	<u>Panel Finding</u>
Culebra Hydrogeology	Adequate*
Repository Fluid Flow	Adequate*
Units Above the Salado	Adequate*
Exploration Boreholes	Adequate*
Spallings	Not Adequate
Direct Brine Release	Adequate*
Castile and Brine Reservoir	Adequate*
Chemical Conditions	Not Adequate

The conceptual models marked with asterisks were judged to be adequate on the basis of no impact on PA. The subsequent review in January 1997 did not alter the Panel's adequacy conclusions.

The Panel met again in April 1997 to review additional DOE information regarding the Spallings and Chemical Conditions Conceptual Models. DOE specifically did not request the Panel to assess the adequacy of the two remaining conceptual models to meet the regulatory requirement. Rather, DOE presented additional information to the Panel, and asked whether, based on this new information, the results predicted by these inadequate conceptual models were "reasonable." The Panel concluded that the Chemical Conditions Model was adequate to meet the regulatory requirement of Section 194.23(a)(3)(i) concerning future states of the repository because:

The additional information for the Chemical Conditions model included further data from the MgO test program regarding hydration of MgO and transition toward magnesite, reaction rates with carbonate species, control of pH, and effect on actinide solubility. The Panel's only remaining concern for this model related to the lack of a demonstrated ability of the MgO backfill to function according to the assumptions in the conceptual models as used in the CCA with respect to reaction with the generated CO₂ gas. The results of the information and analysis are sufficiently complete at this time for the Panel to conclude that the MgO backfill will function as assumed in the CCA and that this model is adequate to represent the future states of the repository. (Docket A-93-02, Item II-G-22, pp. 17-18)

The Panel did not conclude that the Spallings Model is adequate to meet the regulatory requirement of Section 194.23(a)(3)(i). Nonetheless, the Panel found that released volumes estimated in the CCA were deemed reasonable and "may actually overestimate" the actual released waste volumes (Docket A-93-02, Item II-G-22). With the exception of the Spallings Model, the Panel stated "all remaining conceptual models have been determined to be adequate and all significant issues regarding their adequacy have been resolved" (Docket A-93-02, Item II-G-22).

7.4 EPA COMPLIANCE REVIEW

All conceptual models used in the CCA were the subject of peer review by the Conceptual Models Peer Review Panel. The peer review process was iterative in nature, with additional information provided by DOE to support the models initially judged by the Panel to be inadequate. The peer review process was documented sufficiently to show the subsystem components that were evaluated and the results of the peer review. EPA found that the Conceptual Models Peer Review was conducted in accordance with the peer review requirements of Section 194.27 (see **CARD 27—Peer Review** for further information). Based upon the information available in Appendix PEER, EPA determined that the Panel had access to sufficient information to evaluate data and information used to develop conceptual models, the validity of assumptions, alternate conceptual models, and uncertainty in the conceptual models, including consequences if the conceptual model chosen is inappropriate. The Panel stated the adequacy of the conceptual models and the accuracy of the results from those models, and the Panel discussed the validity of the conclusions drawn based on the conceptual models. Therefore, EPA found the conclusions of the Conceptual Models Peer Review Panel to be reliable and sufficient.

All models were eventually judged to be adequate for use in PA either on the basis of total acceptability, acceptability based on no significant impact on PA or, in the case of spallings, acceptability based on conservative results. The Conceptual Models Peer Review Panel found that the final conceptual model(s) and the subsystem components used in the compliance application represented a reasonable approximation of the actual disposal system. EPA agreed with the peer review panel that all models but the spalling model are adequate for use in the PA calculations. EPA also agreed with the panel's finding in its third report that the results of the spallings model are reasonable for use in the PA calculations, and that they may even overestimate releases, because the far more realistic alternate modeling presented by DOE to the Panel predicted releases far below those predicted by the original spallings model used in the PA calculations (Docket A-93-02, Item II-G-22). Thus, for purposes of determining whether the WIPP will comply with the 40 CFR Part 191 radioactive waste disposal regulations, use of the results from the inadequate spallings model is conservative, and is consistent with EPA's obligation to have a rational basis for its determination.

During the public comment period on EPA's proposed certification decision, the Agency received many comments related to the adequacy of the spallings conceptual model. These included comments on DOE's treatment of spallings in the CCA, DOE and EPA's other spallings analyses, and DOE's decision to model only the "blowout" spallings mechanism and not "stuck pipe" or "gas erosion" mechanisms. None of these comments challenged the procedures used by the Conceptual Models Peer Review Panel. EPA completed an additional analysis of spallings due to air drilling in response to public comments; see EPA's Analysis of Air Drilling at WIPP (Docket A-93-02, Item IV-A-1). For a general discussion of these issues and EPA's responses, see the "Modeling and Performance Assessment" section of the preamble. For a detailed discussion of these issues, see the EPA Response to Comments, Section 5. Refer to sections on General Spallings Comments, Stuck Pipe, Gas Erosion and Related Waste Permeability, and SNL/DOE's Spallings GASOUT Computer Code.

8.0 REQUIREMENT

(b) “Computer codes used to support any compliance application shall be documented in a manner that complies with the requirements of ASME NQA-2a-1990 addenda, part 2.7, to ASME NQA-2-1989 edition.”

8.1 ABSTRACT

CARD 22—Quality Assurance, under the discussion of Section 194.22(a)(2)(iv), explains how EPA verified that the development of DOE’s computer codes for the PA and compliance assessment adhere to the quality assurance requirements specified in Section 194.22, and that DOE’s documentation was consistent with the requirements of ASME NQA-2a-1990 addenda, part 2.7. EPA required additional information demonstrating that DOE documented computer codes in accordance with the relevant quality assurance standards. EPA found that DOE’s quality assurance requirements for the PA and compliance assessment were in agreement with those specified in Section 194.22, and that their code documentation was adequate. DOE’s QA documentation includes plan(s) for quality assurance software, software requirements documentation, software design and implementation documentation, software verification and validation documentation, and user documentation.

8.2 COMPLIANCE REVIEW CRITERIA

EPA expected information in the CCA to be consistent with the quality assurance requirements of ASME NQA-2a-1990 addenda, part 2.7, to ASME NQA-2-1989 edition. This documentation should contain plan(s) for quality assurance software, software requirements documentation, software design and implementation documentation, software verification and validation documentation and user documentation.

8.3 DOE METHODOLOGY AND CONCLUSIONS

Chapter 5 of the CCA discusses DOE’s quality assurance (QA) program. Discussion of software QA is provided in Chapter 5.1.4 and 5.3.20 (pp. 5-7 to 5-10 and 5-40 to 5-41). The CAO Quality Assurance Program Document (CAO QAPD), dated April 22, 1996, is contained in Appendix QAPD. The CAO QAPD incorporates the requirements of ASME NQA-2a-1990 addenda, part 2.7, to ASME NQA-2-1989 edition, Section 6. See **CARD 22—Quality Assurance**, requirements Section 194.22(a)(1) and (a)(2)(iv), for further discussion of DOE’s approach to the quality assurance requirements for computer codes and models.

8.4 EPA COMPLIANCE REVIEW

EPA verified compliance with the requirements of Section 194.22(a)(2)(iv) by reviewing Section 6.0 of the CAO QAPD and conducting audits of the SNL and Westinghouse’s Waste Isolation Division quality assurance programs. DOE’s documentation includes plan(s) for software quality assurance, software requirements documentation, software design and implementation documentation, software verification and validation documentation and user

documentation. EPA notified DOE by letter that the CCA did not document computer codes in a manner consistent with the standards (Docket A-93-02, Item II-I-01). DOE submitted the required documentation in supplementary materials, including QA packages for 13 PA Codes (Docket A-93-02, Item II-G-03). EPA found that DOE's quality assurance requirements for computer codes used in the PA and compliance assessment were in agreement with those specified in Section 194.22, and that their code documentation was adequate. See **CARD 22—Quality Assurance**, requirements Section 194.22(a)(1) and (a)(2)(iv), for further discussion of EPA's compliance review of the quality assurance requirements for computer codes and models.

9.0 REQUIREMENT

(c) "Documentation of all models and computer codes included as part of an compliance application performance assessment calculation shall be provided. Such documentation shall include, but shall not be limited to:

(1) Descriptions of the theoretical backgrounds of each model and the method of analysis or assessment."

9.1 ABSTRACT

EPA evaluated whether DOE's descriptions of the theoretical backgrounds for the computer codes in the CCA provided sufficient detail to allow a thorough technical assessment. EPA also evaluated whether the CCA contained documentation describing exactly how each of the codes was used to support the PA. The information that EPA reviewed was primarily contained in User's Manuals, Validation Documents, Implementation Documents, and Requirements Document & Verification and Validation Plans for each code (referenced in EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 9.0, Docket A-93-02, Item V-B-6). The most relevant information related to these issues is found in the User's' Manuals and Analysis Packages for each code (see Docket A-93-02, Item II-G-3, Volumes 1 to 12 for each computer code). The codes that EPA reviewed include: CUTTINGS_S, SECOFL2D, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO_DBR, NUTS, FMT, GRASP-INV, SANTOS and ALGEBRA. In a few cases, EPA initially found the theory describing aspects of the computer codes to be inadequate. Most notably, the mathematical description of the precipitation model contained in the NUTS code, which predicts radionuclide transport in units underlying the Culebra, was absent from the documentation (see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 9, Docket A-93-02, Item V-B-6). DOE rectified EPA's concerns by issuing supplementary reports that describe in detail those theoretical discussions that were originally deficient, in addition to other deficient information related to documentation of codes (see Docket A-93-02, Items II-I-02 to II-I-38 for DOE responses to EPA letters). With respect to the documentation pertaining to the method of analysis, EPA found the descriptions in the Analysis Packages for each code to be sufficiently complete. In several instances, EPA requested that DOE clarify the written documentation, which DOE subsequently provided.

9.2 COMPLIANCE REVIEW CRITERIA

EPA reviewed all available documentation for each of the computer codes for completeness, clarity, and logical development of the theoretical bases of the conceptual models used in each computer code. Documentation was considered complete if it contained sufficient information from which to judge whether the codes were both formulated on a sound theoretical foundation and used properly in the PA analysis.

9.3 DOE METHODOLOGY AND CONCLUSIONS

See the Background section of this CARD for a discussion of how conceptual models provide theoretical background that is incorporated into computer codes. DOE's documentation of conceptual models, alternative conceptual models, and the Conceptual Models Peer Review Panel is discussed above in this CARD in the DOE Methodology discussion for the requirements of Section 194.23 (a)(1), (a)(2) and (a)(3)(v). Information regarding whether the computer codes satisfied the requirements of Section 194.23(c)(1) is contained in the documents described below for each modeling code (see Docket A-93-02, Item II-G-3, Volumes 1 to 12 for each computer code). DOE indicated that the major codes modeling the repository and its surroundings are CUTTINGS_S, SECOFL2D, SECOTP2D, CCDFGF, PANEL, BRAGFLO, BRAGFLO_DBR, NUTS, FMT, GRASP-INV, and SANTOS (Chapter 6.4.11, pp. 6-173 to 6-180). In addition, LHS and ALGEBRA perform critical functions of sampling of parameters and initializing data in order to run PA computer codes.

- ◆ User's Manual (UM)—describes the code's purpose and function, mathematical governing equations, model assumptions, the user's interaction with the code, and the models and methods employed by the code. The User's Manual generally includes:
 - The numerical solution strategy and computational sequence, including program flowcharts and block diagrams.
 - The relationship between the numerical strategy and the mathematical strategy (i.e., how boundary or initial conditions are introduced).
 - A clear explanation of model derivation. The derivation starts from generally accepted principles and scientifically proven theories. The User's Manual justifies each step in the derivation and notes the introduction of assumptions and limitations. For empirical and semi-empirical models, the documentation describes how experimental data are used to arrive at the final form of the models. The User's Manual clearly states the final mathematical form of the model and its application in the computer code.

- Descriptions of any numerical method used in the model that goes beyond simple algebra (e.g., finite-difference, Simpson's rule, cubic splines, Newton-Raphson Methods, and Jacobian Methods). The User's Manual explains the implementation of these methods in the computer code in sufficient detail so that an independent reviewer can understand them.
 - The derivation of the numerical procedure from the mathematical component model. The User's Manual gives references for all numerical methods. It explains the final form of the numerical model and its algorithms. If the numerical model produces only an intermediate result, such as terms in a large set of linear equations that are later solved by another numerical model, then the User's Manual explains how the model uses intermediate results. The documentation also indicates those variables that are input to and output from the component model.
- ◆ Analysis Packages (AP)—contain detailed information on how the computer codes were used in the PA, including code implementation approaches and justification of parameters used. DOE required its code User's to supply the following information relevant to Section 194.23(c)(1) in its Analysis Packages:
- Description of the overall nature and purpose of the general analysis performed by the model. The Analysis Packages state the specific aspects of the analysis for which the model is used. The documentation shows input and output parameters of the model. The Analysis Packages discuss the input and output parameters for each model.
 - The modeling information describing the components (e.g., unsaturated vs. saturated) and their role in the overall modeling effort. The Analysis Packages identify the contribution of each component model to the complete solution of the problem and the linkages between the component models. The documentation uses flowcharts and block diagrams to describe the mathematical solution strategy for the PA.

DOE used three additional documents as secondary references:

- ◆ Requirements Document & Verification and Validation Plan (RD/VVP)—a single document that identifies the computational requirements of the code (e.g., SECOFL2D must be able to simulate ground water flow under steady-state conditions). The RD/VVP also describes how the code will be tested to ensure that those requirements are satisfied.

- ◆ Implementation Document (ID)—provides the information necessary for the recreation of the code used in the 1996 WIPP PA calculation. Using this information, the computer user can reconstruct the code or install it on an identical platform to that used in the 1996 WIPP PA calculation. The document includes the source-code listing, the subroutine-call hierarchy, and code compilation information as discussed in the EPA Technical Support Document for Section 194.23: Models and Computer Codes, Appendix A (Docket A-93-02, Item V-B-6).

- ◆ Validation Document (VD)—Summarizes the results of the testing activities prescribed in the Requirements Document and Verification and Validation Plan documents for the individual codes and provides evaluations based on those results. The Validation Document contains listings of sample input and output files from computer runs of a model. The Validation Document also contains reports on code verification, benchmarking, and validation, and also documents results of the quality assurance procedures. For more information on these activities, see the EPA Technical Support Document for Section 194.23: Models and Computer Codes, Appendix A (Docket A-93-02, Item V-B-6).

In general, a set of these five documents exists for each of the codes (see Docket A-93-02, Item II-G-3, Volumes 1-12, for each computer code). DOE used these documents as the primary vehicles to describe the conceptual models, mathematical models, and numerical methods that provide the basis for the theory and the assumptions underlying the computer codes. DOE included additional documentation in various appendices to the CCA (e.g., BRAGFLO, SECOTP). DOE's documentation also contains justification for the use of the models, the conceptual model derivation, the mathematical derivations, and the solution methods used in the codes (referenced in EPA Technical Support Document for Section 194.23: Models and Computer Codes, Appendix A, Docket A-93-02, Item V-B-6).

9.4 EPA COMPLIANCE REVIEW

EPA reviewed all of the relevant documentation pertaining to the theoretical development and application of the models mentioned in Section 9.3 above. For further discussion of EPA's review of documentation of conceptual models, alternative conceptual models, and the Conceptual Models Peer Review Panel, see the "EPA Compliance Review" discussions for the requirements of Section 194.23 (a)(1), (a)(2), and (a)(3)(v) above in this CARD. The majority of the information was located in the User's Manuals and Analysis Packages for each code. During EPA's review, EPA identified a number of areas where the documentation was not adequate to allow a technical evaluation of the theoretical mathematical formulations or modeling approach. For example, EPA required DOE to submit testing documentation of the SECO3D code (Docket A-93-02, Item II-I-01). In addition, EPA required additional theoretical discussion of the NUTS and SECO computer codes; see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 9.4 (Docket A-93-02, Item V-B-6) and Docket A-93-02, Items II-I-01 and II-I-17.

In most instances, DOE was able to clarify these issues satisfactorily in their responses to EPA's comments; see Section 9.0 of EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6) and Docket A-93-02, Item II-I-31. After further informal clarification from EPA, DOE issued additional supporting documentation filed at Docket A-93-02, Items II-G-17, II-G-18, II-I-02, II-I-03, II-I-07, II-I-08, II-I-10, II-I-16, II-I-19, II-I-24, II-I-28, II-I-30, II-I-34, II-I-35, II-I-36, and II-I-38. As discussed in Section 9.1 of EPA Technical Support Document for Section 194.23: Models and Computer Codes, EPA continued to request additional information and studies until EPA was satisfied that the descriptions of the theoretical backgrounds of each model and the method of analysis were reasonable.

EPA found that DOE's level of documentation was consistent with the ASME requirements for quality assurance and also with recent standards on ground water modeling published by the American Society for Testing and Materials (ASTM). ASTM is a private organization that publishes consensus standards for a variety of fields, including ground water modeling. The ASTM Subcommittee D18.21 on Ground water and Vadose Zone Investigations has approved six new standards related to ground water modeling. These standards have been written in the form of guidance and are referenced in Section 9.4 of the EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6).

10.0 REQUIREMENT

(c) "Documentation of all models and computer codes included as part of a compliance application performance assessment calculation shall be provided. Such documentation shall include, but shall not be limited to:

(2) General descriptions of the models; discussions of the limits of applicability of each model; detailed instructions for executing the computer codes, including hardware and software requirements, input and output formats with explanations of each input and output variable and parameter (e.g., parameter name and units); listings of input and output files from a sample computer run; and reports on code verification, bench marking, validation, and quality assurance procedures."

10.1 ABSTRACT

Information regarding DOE's compliance with Section 194.23(c)(2) is primarily contained in User's Manuals (UM), Analysis Packages (AP), Validation Documents (VD), Implementation Documents (ID), and Requirements Document & Verification and Validation Plans (RD/VVP) for each code. The codes that EPA reviewed include: CUTTINGS_S, SECOFL2D, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO_DBR, NUTS, FMT, GRASP-INV, SANTOS and ALGEBRA. Table 3 lists the requirements of 194.23(c)(2) and where these requirements are documented in DOE documents. EPA determined that DOE documents fulfilled the requirements of 194.23(c)(2) after reviewing these documents, executing the computer codes, and evaluating the code verification, bench marking, and validation documentation.

10.2 COMPLIANCE REVIEW CRITERIA

EPA expected the CCA to include:

- ◆□ A general description of each model used in the calculations.
- ◆□ A description of the limits of applicability of each model.
- ◆□ Detailed instructions for executing the computer codes.
- ◆□ Hardware and software requirements to run these codes.
- ◆□ Input and output formats with explanations of each input and output variable and parameter.
- ◆□ Listings of input and output files from sample computer runs.
- ◆□ Reports of code verification, bench marking, validation, and quality assurance procedures.

EPA also expected the CCA to describe any limiting assumptions or conditions placed on each model in sufficient detail to allow a reviewer to understand their impact on the performance and accuracy of model results. EPA expected that reports of QA procedures would meet the quality assurance criteria outlined in Sections 4 and 6 of the ASME NQA-2a-1990 addenda, part 2.7, to ASME NQA-2-1989.

10.3 DOE METHODOLOGY AND CONCLUSIONS

See the Background section of this CARD for a discussion of how conceptual models, mathematical models, and numerical models are used to develop computer codes. The information that EPA relied upon in its determination of whether DOE satisfied the requirements of Section 194.23(c)(2) is primarily contained in the UM, AP, VD, ID, and RD/VVP for each computer code. See “DOE Methodology” under Section 194.23(c)(1) above for descriptions of these documents.

A set of these five documents exists for each major code, except the SANTOS computer code. DOE used these documents as the primary vehicles to provide the information required by Section 194.23(c)(2). Table 3 indicates the documents in which DOE provided the required information. DOE set forth a number of objectives regarding issues that must be covered in their documentation to meet the quality assurance criteria outlined in Sections 4 and 6 contained in the ASME NQA-2a-1990 addenda, part 2.7, to ASME NQA-2-1989.

10.4 EPA COMPLIANCE REVIEW

EPA reviewed all of the relevant documentation pertaining to the requirements specified in Section 194.23(c)(2) for the following codes: CUTTINGS_S, SECOFL2D, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO_DBR, NUTS, FMT, GRASP-INV, SANTOS and ALGEBRA. EPA identified numerous deficiencies regarding these requirements. These deficiencies are identified in letters to DOE requiring the submission of specific information (Docket A-93-02, Items II-I-01 and II-I-17). For example, DOE was required to perform a mass balance analysis on the NUTS computer code, develop a code requirement for transmissivity field simulations, and test the end-to-end statistical validity of these simulated transmissivity fields in order to provide the probabilistic inputs for the PA. In addition, EPA required DOE to provide evidence that the GRASP-INV code was tested in the manner in which it was implemented in the PA and a sample computer run that corresponds to the CCA results.

DOE provided additional supporting documentation that satisfied all of the deficiencies identified by EPA (see Docket A-93-02, Items II-G-17, II-G-18, II-I-16, and II-I-19.) Specifically, DOE provided documentation showing that DOE: performed a mass balance on the NUTS computer code; developed a code requirement for transmissivity field simulations and tested the statistical validity of these simulations; tested the implementation of the GRASP-INV code consistent with its implementation in the PA; and provided a sample computer run corresponding to the PA results. DOE's documentation provided enough information to allow EPA to understand and execute the models, to determine the possible impact of any assumptions, and to verify that the codes were tested and quality assured. EPA therefore determined that the documentation was sufficient for the requirements of Section 194.23(c)(2).

11.0 REQUIREMENT

(c) "Documentation of all models and computer codes included as part of a compliance application performance assessment calculation shall be provided. Such documentation shall include, but shall not be limited to:

(3) Detailed descriptions of the structure of the computer codes and complete listings of the source codes."

11.1 ABSTRACT

The relevant information for meeting the requirements of Section 194.23(c)(3) is primarily contained in the Implementation Document(s) for each code. The codes that EPA reviewed include: CUTTINGS_S, SECOFL2D, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO_DBR, FMT, NUTS, GRASP-INV, SANTOS and ALGEBRA. DOE submitted all of the source code listings in the Implementation Documents and EPA identified no problems with the descriptions of the structure of the computer codes.

**Table 3
Location of Documentation for Models and Computer Codes
Used in Performance Assessment**

Requirement in Compliance Application Guidance	Document Containing Information					
	User's Manual	Analysis Packages	Validation Document	Implement-ation Document	Requirements Document & Validation and Verification Plan	SNL QA Procedures*
General descriptions of the models	✓☐					✓☐
Discussions of the limits of applicability of each model	✓☐					✓☐
Detailed instructions for executing the computer codes		✓☐		✓☐		✓☐
Hardware requirements for executing the computer codes	✓☐	✓☐		✓☐		✓☐
Software requirements for executing the computer codes	✓☐					✓☐
Input and output formats with explanations of each input and output variable and parameter	✓☐	✓☐				✓☐
Listings of input and output files from a sample computer run	✓☐					✓☐
Reports on code verification			✓☐		✓☐	✓☐
Reports on bench marking			✓☐		✓☐	✓☐
Reports on validation			✓☐		✓☐	✓☐
Reports on quality assurance procedures						✓☐

✓☐ = Information meeting the requirement is found in this document.

* = See CCA Appendix QAPD, Section 6.0.

11.2 COMPLIANCE REVIEW CRITERIA

EPA expected the CCA to contain a detailed description of the structure of the computer codes. DOE must submit the source code listing and accompany it with a detailed description of the code structure. EPA also expected the documentation of computer codes to describe the structure of computer codes with sufficient detail to allow EPA to understand how software subroutines were linked and how the code structure operates to provide accurate solutions of the conceptual models.

11.3 DOE METHODOLOGY AND CONCLUSIONS

The information relevant to compliance with Section 194.23(c)(3) was contained in the Implementation Document for each modeling code (see Docket A-93-03, Item II-G-3, Volumes 1-12, for each computer code). This document provided the information necessary for the recreation of the code as used in the 1996 WIPP PA calculation. With this information the user can compile the source code and install it on a computer system identical to that used in the 1996 WIPP PA calculation. The document includes the source-code listing, the subroutine-call hierarchy, and code compilation information.

11.4 EPA COMPLIANCE REVIEW

EPA reviewed all of the relevant documentation, in particular the ID for each computer code pertaining to the requirements specified in Section 194.23(c)(3) for the following codes: CUTTINGS_S, SECOFL2D, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO_DBR, NUTS, FMT, GRASP-INV, SANTOS and ALGEBRA. EPA found that DOE submitted all of the source code listings. EPA identified no problems with the detailed descriptions of the structure of the computer codes. The documentation of computer codes described the structure of computer codes with sufficient detail to allow EPA to understand how software subroutines were linked.

12.0 REQUIREMENT

(c) "Documentation of all models and computer codes included as part of a compliance application performance assessment calculation shall be provided. Such documentation shall include, but shall not be limited to:

(4) Detailed descriptions of data collection procedures, data reduction and analysis, and code input parameter development."

12.1 ABSTRACT

DOE discussed information supporting parameter development in the CCA and related documents. EPA reviewed Chapter 6.0, Appendix PAR, and parameter records located in the SNL WIPP Record Center. The parameter records at SNL Record Center include WIPP parameter entry forms (464 Forms), Parameter Records Packages (PRP), Principal Investigator

Records Packages (PIRP), Data Records Packages (DRP), and Analysis Packages (AP). EPA reviewed parameter documentation and record packages for approximately 1,600 parameters used as input values to the PA calculations. Initially, EPA identified concerns in three areas: the completeness of the list of 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.

DOE improved documentation in the SNL Record Center for records that justify the source of parameters. DOE also developed better “roadmaps” to link parameter documentation and parameter development. Upon review and evaluation of this supplementary information, EPA determined that DOE had: improved records in the SNL Record Center; adequately provided a detailed listing of the code input parameters; listed input parameters sampled; 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 and an explanation of quality assurance activities.

EPA’s detailed review of the parameters used in the PA calculations can be found in the following EPA Technical Support Documents for Section 194.23: Parameter Report (Docket A-93-02, Item V-B-12), Sensitivity Analysis Report (Docket A-93-02, Item V-B-13), and Parameter Justification Report (Docket A-93-02, Item V-B-14).

12.2 COMPLIANCE REVIEW CRITERIA

EPA expected DOE to provide:

- ◆□ 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 parameters development.
- ◆□ Discussion of the linkage between input parameter information and data used to develop the input information.
- ◆□ Discussion of the importance of the sampled parameters relative to final releases, correlations among sampled parameters, and how these are addressed in PA.

- ◆ A listing of the sources of data used to establish parameters (e.g., experimentally derived, standard textbook values, and results of other computer codes).
- ◆ Data reduction methodologies used for PA parameters used in the calculations, including an explanation of quality assurance activities (see 194.22(a)(2)(iv) in **CARD 22—Quality Assurance** for EPA’s review of DOE’s QA activities for parameters and code development).

12.3 DOE METHODOLOGY AND CONCLUSIONS

The primary sources of parameter information are CCA Chapter 6 (especially Tables 6-8 to 6-27, pp. 6-101 to 6-166), Appendix PAR, and other appendices describing specific computer codes and parameter records in the SNL Record Center (see Section 17 of this CARD). Records in the SNL Record Center that EPA used to evaluate parameters include:

- ◆ SNL Form 464, WIPP Parameter Entry Form: All PA parameters are defined using this form, which contains the numerical values and distributions of parameters used as input to PA codes, identifies the code the parameter is used in, and includes information to trace the development of each parameter.
- ◆ Parameter Records Packages (PRP): The PRP provides information used in Form 464 and provides additional depth regarding the parameter’s development, derivation, and documentation. The PRP explains the final development and data reduction of a set of measured values into a form that a PA computer code can use.
- ◆ Principal Investigator Records Packages (PIRP): PIRPs document parameters that involve considerable data reduction and analysis by the SNL Principal Investigator or other technical personnel. The PIRP is the second step of PA parameter development. Data reduction and analysis are usually explained at this step.
- ◆ Data Records Packages (DRP): These documents are typically generated for parameters that are derived from empirical testing as a result of laboratory or field measurements (for example, actinide solubility experiments or brine inflow rate measurements in the WIPP underground). These packages are generally the first step that links the development of a parameter from the measured data to the values used in the PA.
- ◆ Analysis Packages (AP): These are supplementary documents that generally describe all parameters used by a particular code in the PA calculations and typically describe the development of “legacy” parameters

(i.e., parameters with values that previously were used in the 1992 PA); see Docket A-02-93, Items II-G-04 to II-G-11).

Documentation for each parameter began with Form 464. The need for further documentation in the other four types of documents depended upon the nature of the parameter, such as whether it is a widely accepted chemical constant (e.g., atomic weight of an isotope), or whether it is a value requiring experimental data for verification. See EPA Technical Support Document for Section 194.23: Parameter Report for specific parameter record information (Docket A-93-02, Item V-B-12). Figure 2 below describes the types of information found in each of these five documents and possible paths in documenting parameter record information.

Approximately 1,600 parameters provide numerical values or ranges of numerical values 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. Some parameters are well-established chemical constants, such as Avogadro's Number or the Universal Gas Constant. Other parameters describe attributes unique to the WIPP, such as the solubility and mobility of specific actinides in brines in the WIPP. An example of a parameter related to the geology of the WIPP is the permeability of the rock in the Culebra dolomite member of the Rustler Formation above the WIPP. DOE also assigned parameters to consider the effects of human intrusion, such as the diameter of a drill bit used to drill a borehole that might penetrate the repository.

Using the documents described above, DOE describes the methods that develop and support the approximately 1,600 parameters used in the PA calculations (see EPA Technical Support Document for Section 194.23: Parameter Report, Docket A-93-02, Item V-B-12 for details). All of the documents listed above are used to explain the full development of parameter values used as inputs to the PA calculations. Table 4 indicates the documents that contain information required under Section 194.23(c)(4).

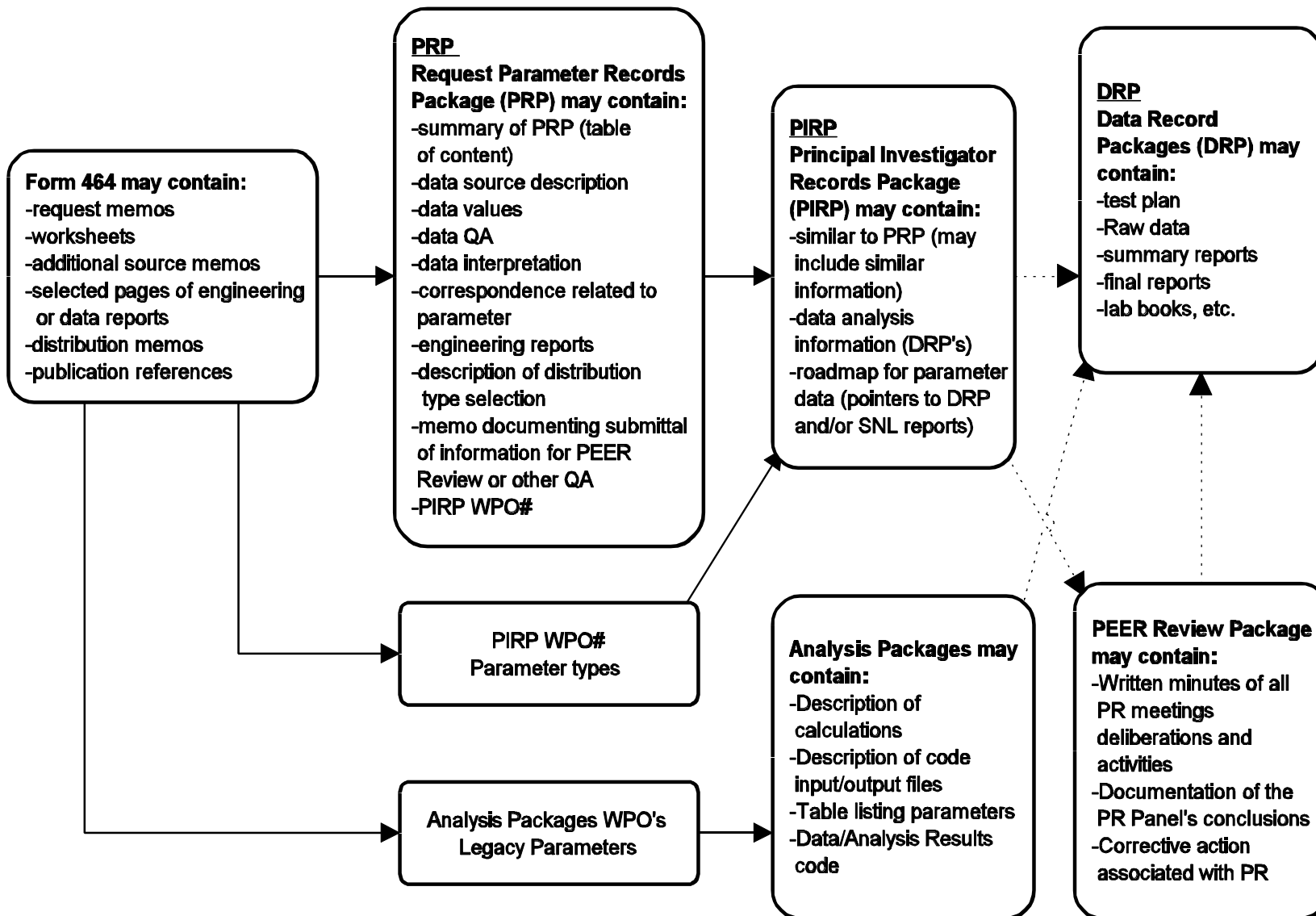


Figure 2: Parameter Documentation

12.4 EPA COMPLIANCE REVIEW

EPA Parameter Review

EPA performed a thorough review of the parameters and the parameter development process. EPA's review of the parameters and parameter development is described in detail in Section 12.0 of EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-6) and in EPA Technical Support Document for Section 194.23: Parameter Report (Docket A-93-02, Item V-B-12). EPA reviewed parameter packages for approximately 1600 parameters used in the PA calculations. EPA then reviewed in greater detail parameter record packages and documentation for more than 400 parameters that were found to be important to the performance of the disposal system. Records reviewed include Chapter 6, Tables 6-8 to 6-27 (pp. 101-166), Appendix PAR, WIPP parameter entry forms (464 Forms), Parameter Records Packages (PRP), Principal Investigator Records Packages (PIRP), Analysis Packages (AP), and Data Records Packages (DRP). EPA's evaluation included a review of the expectations listed in Section 12.2 above.

EPA first examined the sources of different parametric values used in the computer codes. EPA found that 416 (26.4 percent) of the 1571 parameters used in the PA calculations were well-established constants found in general literature and general engineering knowledge. EPA discovered that DOE derived 887 (56.6 percent) of the parameters from experimental data, either from its own experiments or from journal articles. EPA also found that 89 (5.7 percent) were waste-related parameters derived from the waste inventory report (see CCA Appendix BIR). EPA found that DOE selected the values of 149 (5.9 percent) parameters using professional judgment of its employees. Approximately 194 (12.3 percent) parameters were "legacy parameters" originally used in DOE's 1992 PA and incorporated in the PA (see Docket A-93-02, Item II-I-31, Comment No. 11).

Table 4
Location of Required Information on Parameters Used in Codes for Performance Assessment

Requirement In Compliance Application Guidance	Document Containing Information								
	Form 464 ¹	PRP ²	PIRP ³	DRP ⁴	AP ⁵	CCA, Vol. 1 ⁶	App. PAR ⁷	App. QAPD ⁸	Parameter Database ⁹
Detailed listings of code input parameters									✓□
Detailed listings of the parameters that were sampled									✓□
Codes in which the parameters were used	✓□				✓□				✓□
Computer code names of the sampled parameters	✓□				✓□				✓□
Descriptions of the sources of data	✓□	✓□	✓□	✓□					✓□
Descriptions of the parameters					✓□	✓	✓□		✓□
Descriptions of data collection procedures			✓□	✓□					
Descriptions of data reduction and analysis		✓□	✓□	✓□					
Descriptions of code input parameters 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 releases							✓□		
Discussions of correlations among sampled parameters, and how these are addressed in PA							✓□		
Listing of the sources of data used to establish parameters (e.g., experimentally derived, standard textbook values, and results of other computer codes)	✓□	✓□	✓□	✓□					✓□
Data reduction methodologies used for PA parameters used in the calculations		✓□	✓□	✓□					
Explanation of quality assurance activities						✓		✓□	

✓ = information meeting the requirement is found in this document

Table Endnotes

- ¹ Sandia National Laboratories Form 464, WIPP Parameter Entry Form in SNL Records Center
- ² Parameter Records Packages in SNL Records Center
- ³ Principal Investigator Records Packages in SNL Records Center
- ⁴ Data Records Packages in SNL Records Center
- ⁵ Analysis Packages, Docket A-93-02, Items II-G-04 to II-G-11
- ⁶ See CCA Chapter 6 for parameter descriptions and Chapter 5 for an explanation of quality assurance activities
- ⁷ CCA Appendix PAR
- ⁸ CCA Appendix QAPD
- ⁹ DOE Database of parameters, incorporated into EPA Technical Support Document for Section 194.23: Parameter Report, Appendix A (Docket A-93-02, Item V-B-12)

EPA selected 465 parameters on which to concentrate its analysis. EPA selected parameters to review based on the following criteria:

- ◆□ Parameters that appeared to be important to compliance or seemed to be poorly justified, such as material permeabilities and porosities, particle size, brine reservoir characteristics, pressures, solubilities of actinides, and waste inventory information.
- ◆□ Parameters that control various functions of the PA computer codes that appeared to be important to compliance, such as permeability threshold, and dispersivity characteristics of the Culebra.
- ◆□ Other parameters EPA used to evaluate the overall quality of SNL's document traceability, such as reference constants and general reference values.

The purpose of the parameter review was to verify that DOE's documentation adequately fulfilled the criteria identified in "Compliance Review Criteria" above. For further discussion of EPA's examination of the specific parameters in each category, see EPA Technical Support Document for Section 194.23: Parameter Report (Docket A-93-02, Item V-B-12).

After reviewing the 465 selected parameters, EPA notified DOE by letter that there were three categories of parameters not fully documented in the CCA documents or the SNL WIPP Records Center (Docket A-93-02, Item II-I-17). These categories were: (1) parameters lacking supporting evidence (Enclosure 2); (2) parameters that have supporting records for values other than those selected by DOE (Enclosure 3); and (3) parameters that are not explicitly supported by the relevant data or information (Enclosure 4). Letters to DOE dated April 17, 1997 (Docket A-93-02, Item II-I-25) and April 25, 1997 (Docket A-93-02, Item II-I-27), document the results of EPA's ongoing parameter review.

EPA expressed concern about 58 parameters in all. Of these parameters, EPA found that thirteen lacked supporting evidence, five had records supporting different values, and forty were not explicitly supported by DOE's information. DOE provided additional documentation to support its parameter values in response to EPA's letter during various meetings at SNL from March-May 1997. During these meetings, SNL staff presented additional information to support the parameter value used in the PA calculations. These records have been stored in the SNL WIPP Records Center and are documented on the 464 Forms. EPA found that this information supported twelve of the 58 parameters; see EPA Technical Support Document for Section 194.23: Parameter Justification Report, Sections 3, 4 and 5 (Docket A-93-02, Item V-B-14). EPA conducted a sensitivity analysis on most of the 58 parameters to determine if changing the parameter values would have a significant impact upon the results of computer modeling; see EPA Technical Support Document for Section 194.23: Sensitivity Analysis Report, Executive Summary (Docket A-93-02, Item V-B-13). EPA found that 27 of the 58 parameters had a significant impact on results and that 31 of the 58 parameters did not have a significant impact. EPA did not agree with the technical justification of some parameters. EPA could not find adequate documentation to support one of DOE's professional judgment parameters, i.e., the particle diameter value used in the CUTTINGS_S computer code to calculate the spalling release. Other parameters, such as legacy and professional judgment parameters, were found to have

adequate documentation to support the value used in the PA calculations (see EPA Technical Support Document for Section 194.23: Parameter Report, Attachment SR, Docket A-93-02, Item V-B-12).

Verification of Parameter Values and Performance Assessment Verification Test

EPA later required DOE to perform additional PA calculations in a Performance Assessment Verification Test (PAVT) in order to verify that the cumulative impact of all potential problems in codes, parameters, and assumptions incorporated in PA would be small enough that the WIPP would meet the containment requirements of Section 191.13. EPA required DOE to incorporate 24 of the 58 parameters of concern from EPA's list, because either DOE had provided adequate documentation or EPA found that results were insensitive to changes in the parameter for the remaining 34 parameters. The parameters that EPA mandated to be changed for the PAVT are listed in Table 5 below (Docket A-93-02, Item II-G-26). EPA found the original parameters inadequate for a number of reasons. These parameters include 19 of the 24 that are important to results and four parameters for which EPA did not agree with the technical approach taken by DOE (e.g., Castile brine pocket volume derivation); see EPA Technical Support Document for Section 194.23: Parameter Justification Report, Sections 3, 4 and 5 (Docket A-93-02, Item V-B-14). Upon subsequent review, EPA found that parameter number #3259, BLOWOUT, APORO was not actually used in the PA calculations.

The PAVT was run using the new values for the parameters listed in the table below. The ID number, the material name, and the parameter name are identification information used in DOE's records of parameter development. The distribution type, minimum value, maximum value, median value, mean value, and standard deviation characterize the size and shape of the range of values for a parameter. For a comparison of the values of these parameters in the PAVT to the values of these parameters in the CCA PA, see Table ES-4 in EPA Technical Support Document for Section 194.23: Parameter Justification Report (Docket A-93-02, Item V-B-14). Of these parameters, the ones with the most potential for a significant impact on the results of PA are: CASTILER, COMP_RCK, Castile rock bulk compressibility, which impacts the size of the Castile brine pocket which has a major impact on releases; TAUFAIL, the waste shear strength, which impacts how much waste may be released upon impact by a drill bit; and SOLCIM and SOLSIM, solubilities of different radionuclides in the waste depending upon their oxidation state, which affect how much of an actinide is dissolved in brine and then transported.

The PAVT showed that calculated releases may increase by up to three times the mean releases calculated in the original PA and the WIPP will still perform well below the containment requirements at Section 191.13. For further information about the results of the PAVT, see the discussion of requirements 194.34(e) and (f) in **CARD 34—Results of Performance Assessments** and Sections 5 and 6 of EPA Technical Support Document: Overview of Major Performance Assessment Issues (Docket A-93-02, Item V-B-5).

Table 5
EPA Mandated Performance Assessment Verification Testing Parameters

ID No.	Material	Parameter	Distribution Type/Unit	Min	Max	Med	Mean	Standard Dev.
198	DRZ_1	PRMX_LOG	Loguniform/m ²	3.98 x 10 ⁻²⁰	3.16 x 10 ⁻¹³	1.12 x 10 ⁻¹⁶	1.99 x 10 ⁻¹⁴	5.24 x 10 ⁻¹⁴
3184	BH_SAND	PRMX_LOG	Loguniform/m ²	5.01 x 10 ⁻¹⁷	1.00 x 10 ⁻¹¹	2.24 x 10 ⁻¹⁴	8.19 x 10 ⁻¹³	7.85 x 10 ⁻¹²
8001	CONC_PLG	PRMX	Uniform/m ²	1.0 x 10 ⁻¹⁹	1.0 x 10 ⁻¹⁷	5.05 x 10 ⁻¹⁸	--	--
663	WAS_AREA	PRMX_LOG	Constant/m ²	2.4 x 10 ⁻¹³	2.4 x 10 ⁻¹³	2.4 x 10 ⁻¹³	2.4 x 10 ⁻¹³	0.00
2131	REPOSIT	PRMX_LOG	Constant/m ²	2.4 x 10 ⁻¹³	2.4 x 10 ⁻¹³	2.4 x 10 ⁻¹³	2.4 x 10 ⁻¹³	0.00
2907	STEEL	CORRMCO2	Uniform/M/S	0.00	3.17 x 10 ⁻¹⁴	1.585 x 10 ⁻¹⁴	1.585 x 10 ⁻¹⁴	9.151 x 10 ⁻¹⁵
61	CASTILER	COMP_RCK	Triangular/log (Pa ⁻¹)	2.00 x 10 ⁻¹¹	1.00 x 10 ⁻¹¹	4.00 x 10 ⁻¹¹	5.333 x 10 ⁻¹¹	1.6997 x 10 ⁻¹¹
3493	GLOBAL	PBRINE	Uniform/None	0.01	0.60	0.305	0.305	0.1703
3256	BLOWOUT	FGE	Uniform/None	1.00	18.1	9.55	9.56	4.9363
27	BOREHOLE	DOMEGA	Cumulative/rad/s	4.20	23.0	7.77	8.63	3.16
3482	AM+3	MKD_AM	Loguniform/m ³ /kg	0.020	0.500	0.100	0.1491	0.1286
3480	PU+3	MKD_PU	Loguniform/m ³ /kg	0.020	0.500	0.100	0.1491	0.1286
3481	PU+4	MKD_PU	Loguniform/m ³ /kg	0.900	20.0	4.243	6.1591	5.141
3479	U+4	MKD_U	Loguniform/m ³ /kg	0.900	20.0	4.243	6.1591	5.141
3475	U+6	MKD_U	Loguniform/m ³ /kg	3.00 x 10 ⁻⁵	3.00 x 10 ⁻²	9.487 x 10 ⁻⁴	4.339 x 10 ⁻³	6.808 x 10 ⁻³
3409	SOLMOD6	SOLSIM	Constant/moles/liter	8.75 x 10 ⁻⁵	8.7 x 10 ⁻⁵	8.7 x 10 ⁻⁵	8.7 x 10 ⁻⁵	0.00
3405	SOLMOD6	SOLCIM	Constant/moles/liter	8.8 x 10 ⁻⁶	8.8 x 10 ⁻⁶	8.8 x 10 ⁻⁶	8.8 x 10 ⁻⁶	0.00
3406	SOLMOD3	SOLSIM	Constant/moles/liter	1.2 x 10 ⁻⁷	1.2 x 10 ⁻⁷	1.2 x 10 ⁻⁷	1.2 x 10 ⁻⁷	0.00
3402	SOLMOD3	SOLCIM	Constant/moles/liter	1.3 x 10 ⁻⁸	1.3 x 10 ⁻⁸	1.3 x 10 ⁻⁸	1.3 x 10 ⁻⁸	0.00
3407	SOLMOD4	SOLSIM	Constant/moles/liter	1.3 x 10 ⁻⁸	1.3 x 10 ⁻⁸	1.3 x 10 ⁻⁸	1.3 x 10 ⁻⁸	0.00
3403	SOLMOD4	SOLCIM	Constant/moles/liter	4.1 x 10 ⁻⁸	4.1 x 10 ⁻⁸	4.1 x 10 ⁻⁸	4.1 x 10 ⁻⁸	0.00

ID No.	Material	Parameter	Distribution Type/Unit	Min	Max	Med	Mean	Standard Dev.
3408	SOLMOD5	SOLSIM	Constant/moles/liter	2.4×10^{-7}	2.4×10^{-7}	2.4×10^{-7}	2.4×10^{-7}	0.00
3404	SOLMOD5	SOLCIM	Constant/moles/liter	4.8×10^{-7}	4.8×10^{-7}	4.8×10^{-7}	4.8×10^{-7}	0.00
3478	TH+4	MKD_TH	Loguniform/m ³ /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 ³	0.50	4.00	2.25	2.25	1.01

Qualification of Parameter Data

EPA reviewed DOE's qualification of parameter data. Section 194.22(b) requires DOE to qualify data and information collected prior to the implementation of the quality assurance program required pursuant to Section 194.22(a)(1). Data may be qualified by peer review, corroborating data, confirmatory testing, or a quality assurance program that is equivalent in effect to ASME NQA-1-1989. Of the 1571 parameters used in the PA calculations, 133 fell into this category. EPA reviewed the results of DOE's qualification process during EPA's parameter review. DOE agreed to include in the PA parameter database two columns to specify the qualification of all parameters used in the PA calculations; see EPA Technical Support Document for Section 194.23: Parameter Report, Appendix A, List of Database Parameters (Docket A-93-02, Item V-B-12). The first column is entitled, "Were the data developed under an NQA-1 Program (Y/N)" and the second column is entitled, "Which methods were used to qualify existing data?" If a particular parameter was not developed using an NQA-1 program, then DOE qualified the parameter by one of the following methods (see EPA Technical Support Document for Section 194.23: Parameter Report, Appendix A, Footnote 5, Methods Used to Qualify Existing Data, Docket A-93-02, Item V-B-12):

- ◆□ Peer Review, sometimes noted as "PEER_REV" in the database listing.
- ◆□ Corroborating data.
- ◆□ Confirmatory testing.
- ◆□ Demonstration that the data were collected under a Quality Assurance Program equivalent to NQA-1 and NQA-3.
- ◆□ Peer-reviewed technical literature—journal articles, conference papers, text books, hand books, etc.
- ◆□ If none of the above methods was used, then the data remain unqualified.

DOE used three peer reviews to qualify existing data not collected under the requirements of Section 194.22(a)(1): Engineered Systems, Natural Barriers, and Waste Form/Disposal Room. The purpose of the Engineered Systems Peer Review was to qualify data related to rock mechanics and shaft seals in the WIPP. The purpose of the Natural Barriers Peer Review was to qualify data related to natural barrier subsystems in the WIPP, such as density and permeability of the Salado and Castile Formations. The purpose of the Waste Form/Disposal Room Peer Review was to qualify data related to the conditions created by waste in the disposal system, such as gas generation and actinide solubility.

In all cases, the panels were able to qualify the data used in parameter development based on the information presented to them by DOE. EPA conducted an audit of DOE's records to verify the adequacy of the peer reviews as data qualification exercises; see Section 194.22(b) in **CARD 22—Quality Assurance** for a discussion of this audit. EPA also examined parameter records at the SNL Records Center in order to determine whether the peer review panels had reviewed the appropriate data and whether DOE had used the resulting qualified data in PA calculations. EPA found that the panels had reviewed the appropriate data and that parameter

record packages adequately demonstrated that data qualified by peer review had been used in PA calculations.

For example, EPA investigated documentation of parameter #61, CASTILER, COMP_RCK; see EPA Technical Support Document for Section 194.23: Parameter Report, Technical Review Form, pp. 1-6, for the Castile Rock Bulk Compressibility (Docket A-93-02, Item V-B-12). EPA reviewed the following:

- ◆ □ Parameter Request Memo (WPO# 35597).
- ◆ □ Parameter Record Package (WPO# 31084).
- ◆ □ Undisturbed Anhydrite Rock Compressibility Parameter Package (WPO# 31186).
- ◆ □ Interpretation of Brine Permeability Tests of Salado Formation at the WIPP: First Interim Report (SAND90-0083).
- ◆ □ Memo from Al Lappin to Record documenting submittal to DOE peer review panel (WPO# 38386, included in Parameter Package).

Based on this review, EPA determined that the peer review panel had been supplied sufficient information to qualify parameter #61 for use in the PA calculations. EPA employed the same approach for the 82 of 465 parameters that were peer reviewed.

EPA initially found that documentation in the following areas needed improvement:

- ◆ A comprehensive database of all parameters used in the WIPP PA.
- ◆ A database of all parameters based on empirical data (i.e., derived from laboratory and field experiments).
- ◆ The “roadmaps” that document and link PA parameter development to their sources.
- ◆ The record packages in the SNL Record Center.
- ◆ Those parameters that were used in the PA calculation but had not been changed since the 1992 PA calculations (i.e., legacy parameters).
- ◆ Explanation of why the 149 professional judgment (e.g., code control parameters, physical constants, etc. selected by SNL experts) parameters in the comprehensive parameter database did not require expert elicitation.

As a result of EPA’s letters to DOE dated March 19, 1997 (Docket A-93-02, Item II-I-17), April 17, 1997 (Docket A-93-02, Item II-I-25), and April 25, 1997 (Docket A-93-02, Item II-I-27), DOE worked a number of months to satisfy EPA concerns about documentation listed above. Mainly these activities involved improving the quality of the records stored in the SNL

WIPP Records Center. DOE developed a database of all parameters, which EPA has incorporated in its final parameter report; see EPA Technical Support Document for Section 194.23: Parameter Report, Appendix A (Docket A-93-02, Item V-B-12). DOE also developed a database for empirically-derived parameters, found in Attachment SR-3 of EPA Technical Support Document for Section 194.23: Parameter Report. The Department improved the roadmap of development in the PRP, the PIRP and the DRP (see SNL Parameter Guidebook WPO#47127 at the SNL WIPP Record Center). DOE documented the source of the legacy parameters; see Issue 5 of EPA Technical Support Document for Section 194.23: Parameter Report, Attachment SR.

EPA examined DOE's 149 professional judgment parameters. Of these 149 parameters, EPA accepted 148 on the basis of information contained in Issue 6, Attachment SR, of EPA Technical Support Document for Section 194.23: Parameter Report (Docket A-93-02, Item V-B-12). EPA did not accept the professional judgment parameter of particle size and so required DOE to use the process of expert elicitation to develop the value of parameter #3246, BLOWOUT, PARTDIA. EPA agreed that the other 148 professional judgment parameters were appropriate, based upon the application of professional judgment used to interpret technical literature, such as general technical literature and general engineering information. EPA also agreed that these parameters were supported by the data record packages (see EPA Technical Support Document for Section 194.23: Parameter Report, Attachment SR, particularly Issue 6 on professional judgment parameters). After subsequent review and evaluation of the SNL WIPP Record Center records, EPA determined that DOE dealt adequately with all of the requirements listed in Compliance Review Criteria for Section 194.23(c)(4) above.

During the public comment period on EPA's proposed certification decision, the Agency received many comments about parameter values used in the CCA PA and the PAVT. These included comments on the probability of hitting a brine pocket, the permeability⁶ of borehole plugs, the solubility of actinides, and the distribution coefficients (K_d s) for actinide cations⁷. After reviewing public comments, the Agency concluded that the parameter values used in the PAVT were appropriate and were supported. Furthermore, EPA concluded that an additional performance assessment using revised parameter values was not warranted. For a general discussion of these issues and EPA's responses, see the "Modeling and Performance Assessment" section of the preamble. For a detailed discussion of these issues, see the EPA Response to Comments, Sections 3, 5, and 6. In particular, for Section 3, see discussions of Brine Pocket, Brine Pocket Probability, Brine Pocket Characteristics, K_d Tracing Tests, and Shaft Seals; for Section 5, see discussions of Permeability of Borehole Plugs, CCA Parameters and PAVT Parameter Selection, Castile Brine Pocket Reservoirs Comments, and Sensitivity Analysis; and for Section 6, see discussion of Actinide Solubility Comments.

13.0 REQUIREMENT

⁶ Permeability is the degree to which a fluid can enter something.

⁷ Dissolved waste migrating out of a disposal site would migrate as atoms with a positive electrical charge, or cations; in the case of the WIPP, these could be cation species such as Pu^{+4} or U^{+6} . When liquid such as brine carries the cations through sediment or rock, some of the cations become attached to the surface of these solids. Therefore, the cations travel more slowly than the liquid as a whole. The rate of advance of the cation as the liquid migrates can be described with a number called a retardation factor. Distribution coefficients, or K_d s, are used in calculating the retardation factor.

(c) “Documentation of all models and computer codes included as part of a compliance application performance assessment calculation shall be provided. Such documentation shall include, but shall not be limited to:

(5) Any necessary licenses;

13.1 ABSTRACT

No licenses were required to operate the codes essential for the WIPP PA, as stated by DOE in the CCA Regulatory Crosswalk Table (CCA Volume I, p. XWALK-17). All computer codes for the WIPP PA were developed by and programmed by SNL or its contractors as custom software and require no license to execute or use the computer codes documented in the CCA and supplementary materials.

14.0 REQUIREMENT

(c) “Documentation of all models and computer codes included as part of a compliance application performance assessment calculation shall be provided. Such documentation shall include, but shall not be limited to:

(6) An explanation of the manner in which models and computer codes incorporate the effects of parameter correlation.”

14.1 ABSTRACT

User-specified parameter correlations were introduced into the PA calculations using the Latin Hypercube Sampling (LHS) computer program. DOE used two types of parameter correlations, user-specified and induced. User-specified (explicit correlation) parameter correlations are input to the LHS computer code using a correlation matrix (or table). Induced parameter correlations occur as a result of using a sampled parameter in other calculations through a mathematical formula relationship. Of all the parameters, only rock compressibility and permeability were explicitly correlated in the correlation matrix (or table) in the LHS computer code input file in the PA calculations.

When values that are sampled using the LHS computer code are used to calculate other values in the PA calculations, an induced correlation parameter relationship is created. This is the prevalent method of correlation used in the WIPP PA.

EPA determined that parameter correlations were adequately explained in Appendix PAR of the CCA and were adequately incorporated; see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 14.0 (Docket A-93-02, Item V-B-6). EPA also found that the CCA presented an adequate explanation of the manner in which models and computer codes incorporated the effects of parameter correlations.

14.2 COMPLIANCE REVIEW CRITERIA

EPA expected the CCA to provide an adequate discussion of how parameter correlations were incorporated into the PA and an adequate explanation of the mathematical functions used to describe the derived correlation relationship implemented in the PA calculations. Specifically, EPA expected the CCA to include:

- ◆□ A discussion that explains how the effects of parameter correlation were incorporated.
- ◆□ An explanation of the mathematical functions that describe these relationships.
- ◆□ A description of the potential impact on the sampling of uncertain parameters.

EPA also expected the effects of parameter correlation to be documented for both conceptual models and the formulation of computer codes.

14.3 DOE METHODOLOGY AND CONCLUSIONS

DOE implemented parameter correlations in the WIPP PA using the LHS computer code (see Docket A-93-02, Item II-G-3, Volume 8, "LHS User's Manual," for theoretical background). Parameter correlations were defined for only a few sampled parameters (see Appendix PAR). The general methods for addressing parameter correlation were documented in Iman and Shortencarier (1984).

DOE used two types of parameter correlations, which were defined as explicit parameter correlation and induced parameter correlation. Explicit parameter correlations are introduced or prohibited in the LHS computer code by a user-specified relationship (restricted pairing), as described by Iman and Conover (1982). DOE specified three parameter correlations in the PA through this technique. The only user-specified correlations required in the PA LHS computer code input file were related to rock compressibility and permeability for the Halite (salt), marker bed 139, and the Castile formation. For example, rock compressibility and permeability were correlated for the halite (salt), marker bed 139, and the Castile formation using a correlation relationship of -0.99, -0.99, and -0.75 respectively (see Appendix PAR.4, p. PAR-12, and EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 14.0, Docket A-93-02, Item V-B-6).

Induced correlation of parameters is caused in the PA calculations when a parameter sampled in the LHS code is related to other parameters by mathematical formulas used in subsequent computer codes. This was the prevalent method by which parameter correlation was incorporated into the PA calculations. For example, uncertainty in dissolved actinide oxidation states was derived from the LHS computer code calculations by sampling the oxidation state parameter (OXSTAT, parameter ID #3417). The results of this sampling were used by the ALGEBRA code to determine actinide solubilities, which were used in turn to calculate actinide concentrations in the NUTS and PANEL computer codes. For other induced parameter correlations, see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 14.0 (Docket A-93-02, Item V-B-06).

The PA did not correlate certain parameters that influence the transport of actinides in the Culebra formation (i.e., fracture porosity, spacing and transmissivity). Although these parameters often appear to be correlated in media similar to the Culebra dolomite, DOE stated that its approach was consistent with available data and that these parameters are not correlated (Appendix PAR, p. PAR-13). DOE ensured that the statistical selection of uncorrelated parameters did not lead to unrealistic combinations of parameter values by setting reasonable parameter ranges; see EPA Technical Support Document for Section 194.23: Models and Computer Codes, Section 14.0 (Docket A-93-02, Item V-B-06).

14.4 EPA COMPLIANCE REVIEW

EPA's review focused on whether the CCA contained a complete discussion of how parameter correlations were incorporated into the PA, as well as an adequate explanation of the mathematical functions used to describe the correlation implementation in the CCA. EPA concentrated on DOE's methodology for sampling parameters in the LHS computer program. EPA's analysis of the computational aspects of the LHS computer program and functionality tests performed on the LHS computer code to evaluate the performance of the code is discussed in the LHS computer code section of Appendix A of EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-06).

EPA reviewed how the effects were incorporated into the PA by reviewing the LHS User's Manual, which explains how parameter correlation was included in the parameter sample process (Docket A-93-02, Item II-G-3, Volume 8). EPA also reviewed Appendix PAR.4, which discusses the mathematical methods used to incorporate parameter correlation into the PA calculations. Finally, the Agency reviewed supplementary information (Docket A-93-02, Item II-G-07) that documents DOE sensitivity analysis of the parameters sampled in the PA, including a discussion of the impacts of parameter correlations.

15.0 REQUIREMENT

(d) "The Administrator or the Administrator's authorized representative may verify the results of computer simulations used to support any compliance application by performing independent simulations. Data files, source codes, executable versions of computer software for each model, other material or information needed to permit the Administrator or the Administrator's authorized representative to perform independent simulations, and to access necessary hardware to perform such simulations, shall be provided within 30 calendar days of a request by the Administrator or the Administrator's authorized representative."

15.1 ABSTRACT

DOE provided EPA with ready access to computer hardware required to perform independent computer simulations to verify simulations related to the CCA. DOE also provided EPA with access to data files, source codes, and executable computer codes for each model used in the CCA. DOE provided staff to assist EPA and EPA authorized representatives to execute various verification tests and sensitivity analyses with DOE hardware and software. Descriptions of EPA verification tests for the various models are included in Appendix A to EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-

B-6). A description of the Performance Assessment Verification Test that EPA required is found in Section 12.4 of this CARD.

15.2 COMPLIANCE REVIEW CRITERIA

EPA expected DOE to identify points of contact to facilitate the process for EPA to perform independent simulations, to provide ready access to the hardware and software needed to perform simulations related to evaluation of the CCA, and to assist EPA personnel in exercising DOE computer codes.

15.3 DOE METHODOLOGY AND CONCLUSIONS

DOE designated contacts at SNL to assist EPA and EPA contractor personnel in operating the hardware needed to perform independent computer simulations necessary to verify the simulations related to the CCA. SNL used a special configuration management system (CMS) on the Alpha cluster of VAX computers at SNL in Albuquerque which contained all the codes needed to run the PA. The CMS archives all the input files, output files, source code, and executable files of the modeling codes used by DOE in the PA modeling. DOE provided EPA and authorized personnel with unrestricted access to this computer hardware and software.

15.4 EPA COMPLIANCE REVIEW

As described in EPA Technical Support Document for Section 194.23: Models and Computer Codes, Appendix A (Docket A-93-02, Item V-B-06), EPA performed verification tests on all PA computer codes using CCA hardware and software (see Section 8 of EPA Technical Support Document for Section 194.23: Models and Computer Codes, Docket A-93-02, Item V-B-06). These verification tests were originally designed by DOE to test capabilities required of the codes in the RD/VVP. For example, SECOFL2D must be able to simulate ground water flow under steady-state conditions. In some cases, EPA required DOE to perform additional verification tests, which are described in Section 15 of EPA Technical Support Document for Section 194.23: Models and Computer Codes (Docket A-93-02, Item V-B-06). EPA also conducted extensive parameter sensitivity tests using the same system of PA computer codes; see EPA Technical Support Document for Section 194.23: Sensitivity Analysis Report (Docket A-93-02, Item V-B-13). DOE provided assistance in all of this work on a timely basis.

In addition, EPA conducted a full independent simulation of the PA to verify that the combined effect of all necessary changes to input parameters, computer codes, and models did not require new PA runs (see Docket A-93-02, Item II-G-22). DOE provided all necessary materials and support for EPA to conduct this PA verification test.

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II-G-1	Transmittal of DOE/CAO-1996-2184 Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant, containing Vols. I - XXI and References as follows:	10/96
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V&QD - Verification and Qualification Document

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	<p>Vol. 12 SECO FL2D UM-User's Manual for SECOFL2D, Version 3.01ZO, WPO 22329, September 28, 1995 RD&VVP - Requirements Document and Verification and Validation Plan for SECOFL2D Version 3.01ZO VD - Validation Document for SECOFL2D VERSION 3.01ZO ID - Implementation Documentation for SECOFL2D Version 3.01ZO</p> <p>SECOTP2D UM - User's Manual - Version 1.01 for SECOTP2D, Version 1.30 RD&VVP - Requirements Document and Verification and Validation Plan - Version 1.01 for SECOTP2D (Version 1.30) VD - Validation Document for SECOTP2D Version 1.21ZO ID -Implementation Document for SECOTP2D Version 1.21ZO</p>	
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II-G-08	Analysis Package for the Salado Flow Calculations (Task 1) of the Performance Assessment Analysis - WPO #40514, Supporting the Compliance Certification Application	12/20/96

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II-G-09	Analysis Package for the Salado Transport Calculations (Task 2) of the Performance Assessment - WPO #40515, Supporting the Compliance Certification Application	12/23/96
II-G-10	Analysis Package for the CCDF Construction (Task 7) of the Performance Assessment Analysis - WPO #40524, Supporting the Compliance Certification Application	12/20/96
II-G-11	Analysis Package of the Culebra Flow and Transport Calculations (Task 3) of the Performance Assessment Analysis - WPO #40516, Supporting the Compliance Certification Application Analysis - Plan 019	12/11/96
II-G-12	Waste Isolation Pilot Plant - Conceptual Models Supplementary Peer Review Report	12/96
II-G-17	Analysis Package for the BRAGFLO Sensitivity Study, WPO#43593, Revision #1, dated 3/11/97, entitled "Sensitivity of Flow, Transport, and Direct Brine Release to Grid Refinement Using the BRAFGFLO and NUTS Computer Models." (This document is filed with transmittal letter, see A-93-02, II-I-16.)	3/11/97
II-G-18	Analysis of Ground Water Travel Times through Calibrated Transmissivity Fields Generated by GRASP-INV, WPO#44199 (Version 2.01) Revision O, March 1997, with Appendix A - TCSTRIP UTILITY CODE VERIFICATION Rev. O, March 1997, and Appendix B - HDSTRIP UTILITY CODE VERIFICATION Rev O, March 1997 (Transmittal letter filed A-93-02, II-I-19).	3/97
II-G-21	Waste Isolation Pilot Plant - Conceptual Models Second Supplementary Peer Review Report	1/97
II-G-22	Ltr/DOE-CAO/J.A. Mewhinney to EPA/F. Marcinowski transmitting the Final Report, Waste Isolation Pilot Plant, Conceptual Models Third Supplementary Peer Review Report, April 1997	5/8/97

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II-G-23	DOE/CAO - Spalling Release Positions Paper: Description and Evaluation of a Mechanistically Based Conceptual Model for Spall-- prepared by Sandia National Laboratories and Carlsbad Technical Assistance Contractor	5/1/97
II-G-24	DOE - Final Report - Expert Elicitation on WIPP Waste Particle Size Distributions During the 10,000-year Regulatory Post-Closure Period	6/3/97
II-G-25	Sandia National Laboratories - Waste Isolation Pilot Plant - Expedited CCA Activity - WPO #44158 Supplementary Analyses of the Effect of Salt Water Disposal and Waterflooding on the WIPP including: Atch 1: Injection Methods: Current Practices and Failure Rates in the Delaware Basin DOE.WIPP-97-2240, June 1997 Atch 2: Technical Review by Swift, et al of the HARTMAN Scenario: Implications for the WIPP by John Bredehoeft, June 13, 1997 (This document is filed with the transmittal letter at A-93-02, II-I-36.)	6/17/97
II-G-26	Summary of EPA-Mandated Performance Assessment Verification Test (Replicate 1) and Comparison with the Compliance Certification Application Calculations	7/25/97
II-G-28	Supplemental Summary of EPA-Mandated Performance Assessment Verification Test (All Replicates) and Comparison with the Compliance Certification Application Calculations - WPO#46702	8/8/97
II-G-30	Summary of Uncertainty and Sensitivity Analysis Results for the EPA-Mandated Performance Assessment Verification Test - WPO #46912	8/22/97
II-I-01	Ltr from EPA/M. Nichols to DOE/Alvin Alm/Asst Secretary, transmitting comments regarding completeness and technical sufficiency of the Compliance Certification Application	12/19/96

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II-I-02	<p>Ltr/G. Dials/DOE/CAO to EPA/R. Trovato, responding to EPA's Letter of December 19, 1996 to DOE/L. Alm requesting additional CCA documentation. Supplemental information for the Compliance Certification Application (CCA) includes the following:</p> <p><u>Response to EPA Comments, Enclosure 1:</u></p> <ul style="list-style-type: none">a. 194.23(a)(1) Models and Computer Codesb. 194.23(a)(2) Models and Computer Codesc. 194.32(c) Scope of Performance <p><u>Response to EPA Comments, Enclosure 2</u></p> <ul style="list-style-type: none">a. 194.32(a) Scope of Performance	1/17/97
II-I-03	<p>Ltr / DOE/G. Dials to EPA/R. Trovato - second response package to EPA's letter of December 19, 1996 to DOE/A. Alm. Supplemental Information for the Compliance Certification Application (CCA) includes the following:</p> <p><u>Response to EPA Comments Enclosure 1</u></p> <ul style="list-style-type: none">a. 194.14(a)(3) Content of Compliance Certification Applicationb. 194.22(a)(2)(iii) Quality Assurancec. 194.23(a)(3)(i) Models and Computer Codes <p><u>Response to EPA Comments Enclosure 2</u></p> <ul style="list-style-type: none">a. 194.23(a)(1) Models and Computer Codesb. 194.32(e)(3) Scope of Performancec. 194.33(c)(1) Consideration for drilling events in performance assessmentd. 194.53 Consideration of underground sources of drinking water	1/24/97

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Item No.	Title and/or Subject	Date of Document
II-I-07	<p>Ltr/DOE-CAO/G. Dials to EPA/R. Trovato - third response package to EPA's letter of December 19, 1996 to DOE/A. Alm Supplemental Information for the Compliance Certification (CCA) includes the Following:</p> <p><u>Response to EPA Comments, Enclosure 1</u></p> <ul style="list-style-type: none"> a. 194.23(a)(2) Models and Computer Codes b. 194.24(a) Waste Characterization c. 194.41(a) Active Institutional Control <p><u>Response to EPA Comments, Enclosure 2</u></p> <ul style="list-style-type: none"> a. 194.23(a)(1) & 194.23(a)(2) Models and Computer Codes b. 194.23(a)(3)(ii) Models and Computer Codes c. 194.23(a)(3)(iv) Models and Computer Codes d. 194.23(c)(4) Models and Computer Codes e. 194.43(a) Passive Institutional Controls 	2/7/97
II-I-08	<p>Ltr/DO E-CAO/G. Dials to EPA/R. Trovato - fourth response package to EPA's letter December 19, 1996 to DOE/A. Alm. Supplemental information for the Compliance Certification Application (CCA) includes the following:</p> <p><u>Response to EPA Comments , Enclosure 1:</u></p> <ul style="list-style-type: none"> a. 194.14(a)(2) Content of Compliance Certification b. 194.23(c) Models and Computer Codes c. 194.23(c)(2) Models and Computer Codes d. 194.23(c)(3) Models and Computer Codes e. 194.23(c)(6) Models and Computer Codes f. 194.32(a) Scope of Performance Assessment g. 194.32(e) Scope of Performance Assessment h. 194.34(b) Results of Performance Assessment i. 194.42(a) Monitoring 	2/14/97
II-I-09	<p>Ltr/EPA/R. Trovato to DOE-CAO/G. Dials requesting data record packages</p>	2/18/97

17.0 REFERENCES IN AIR DOCKET A-93-02

Item No.	Title and/or Subject	Date of Document
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II-I-10	Ltr/DOE-CAO/G. Dials to EPA/R. Trovato -fifth response package to EPA's letter of December 19, 1996 to DOE/A. Alm. Supplemental Information for the Compliance Certification Application(CCA) includes the following:	2/26/97
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Response to EPA Comments , Enclosure 1:

- a. 194.14(a)(2) Content of CCA
- b. 194.22(a)(2)(iii) Quality Assurance (Models and Computer Codes)
- c. 194.23(a)(3)(ii) Models and Computer Codes
- d. 194.23(a)(3)(iii) Models and Computer Codes
- e. 194.23(a)(3)(iv) Models and Computer Codes
- f. 194.24(c) and 194.24(c)(1) Waste Characterization
- g. 194.24(c)(4) Waste Characterization
- h. 194.24(g) Waste Characterization
- i . 194.25(b)(i) Future State Assumptions
- j. 194.53 Consideration of Underground Sources of Drinking Water

Response to EPA Comments, Enclosure 2

- a. 194.14(a)(2) Content of CCA
- b. 194.23(a)(3)(i) Models and Computer Codes
- c. 194.23(a)(3)(i) Models and Computer Codes
- d. 194.23(a)(3)(iv) Models and Computer Codes
- e. 194.23(c)(2) Models and Computer Codes
- f. 194.34(c) Results of Performance Assessments
- g. 194.44 Engineered Barriers
- h. 194.51 Consideration of Protected Individual

II-I-12	Ltr/DOE-CAO/G. Dials to EPA/R. Trovato, responding to EPA letter of 2/18/97 requesting data record packages	2/27/97
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II-I-16	Ltr/DOE-CAO/G. Dials to EPA/R. Trovato, supplemental response to Enclosure 1, page 8, 40 CFR 194.23(a)(3)(iv) of EPA's letter of December 19, 1997 to DOE/A. Alm. This supplemental information is an Analysis Package for the BRAGFLO Sensitivity Study, WPO#43593, Revision #1, dated 3/11/97, entitled "Sensitivity of Flow, Transport, and Direct Brine Release to Grid Refinement Using the BRAFGFLO and NUTS Computer Models."	3/13/97
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Item No.	Title and/or Subject	Date of Document
II-I-17	<p>Ltr/EPA/R. Trovato to DOE/A. Alm, transmitting comments regarding completeness and technical sufficiency of DOE's Compliance Certification Application w/6 Enclosures as follows: Enclosure 1 - WIPP CCA Technical Issues- 8 pages Enclosure 2 - Key PA Parameters Lacking Supporting Evidence - 1 page Enclosure 3- PA Parameters Where the Record Supports Other Values - 1 page Enclosure 4 - PA Parameters Not Explicitly Supported by Data/Information - 2 pages Enclosure 5 - EPA Quality Assurance Audits: Findings & Observations - 5 pages Enclosure 6 - EPA Peer Review Audit Findings & Observations - 5 pages</p>	3/19/97
II-I-19	<p>Ltr/DOE-CAO/G. Dials to EPA/F. Marcinowski, Supplemental response to Enc. 2, Page 5, 40 CFR 194.23(c)(2) to EPA's letter of Dec. 19, 1996 to DOE/A. Alm. transmitting the Analysis of Ground Water Travel Times through Calibrated Transmissivity Fields Generated by GRASP-INV, WPO#44199 (Version 2.01) Revision O, March 1997, with Appendix A - TCSTRIP UTILITY CODE VERIFICATION Rev. O, March 1997, and Appendix B - HDSTRIP UTILITY CODE VERIFICATION Rev O, March 1997 (This document is filed at A-93-02, II-G-18).</p>	3/14/97

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Item No.	Title and/or Subject	Date of Document
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II-I-24	Ltr/G. Dials/DOE-CAO to EPA/R. Trovato, responding to March 19, 1997 letter to DOE/A/ Alm regarding CCA issues/comments, as follows:	4/15/97
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Comment No. 2 Data Quality Characteristics
 Comment No. 3 E2 After E2 Scenarios
 Comment No. 9 More Information on Permeability and Porosity Versus Pressure Curves
 Comment No. 12 Does DOE want to Include Other than BIR Data?
 Comment No. 13 Adsorption of Actinides for Cuttings/Caving
 Comment No. 14 Details on HYDRAQL code
 Comment No. 15 Uncertainties on Upper and Lower Limits
 Comment No. 16 Detail on Methods of NDA
 Comment No. 17 Support an EPA Audit of WWIS
 Comment No. 19 Contaminant Transport from Brine Flow from a Single Hole

II-I-25	Ltr/EPA/R. Trovato to DOE/CAO/G. Dials, follow-up to EPA letter of March 19, 1997 to DOE/Alm regarding performance assessment input parameters with two enclosures as follows:	4/17/97
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Enclosure 1 - Parameters no longer in question.
 Enclosure 2 - Parameters not representative of the data.

II-I-27	Ltr/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 with two enclosures as follows:	4/25/97
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Encl. 1 - Parameters no longer in question
 Encl. 2 - Parameters and associated input values that EPA requires to be used in DOE's PA Verification Test

II-I-28	Ltr/DOE/CAO/G. Dials, Mgr to EPA/ORIA/R. Trovato - Second Response to EPA's letter of 3/19/97 requesting additional information the WIPP CCA including the following:	5/2/97
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Response to Enclosure 1:

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Item No.	Title and/or Subject	Date of Document
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Response to Comment #10 regarding Models and Computer Codes
 Response to Comments #14, #15, #18 regarding Waste Characterization
 Response to Enclosure 5:
 Response to EPA findings from EPA Audit of CAO, 12/9-13/96
 Response to EPA findings from EPA Audit of SNL, 1/13-24/97
 Response to Enclosure 6:
 Response to EPA findings/observations from EPA Audit of CAO Peer Review, 2/10-12/97

II-I-29	Ltr/EPA/Carol Browner to DOE/F. Pena - Completeness Determination	5/16/97
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II-I-30	Ltr/DOE-CAO/G. Dials to EPA/R. Trovato transmitting report of DOE's Expert Elicitation on Waste Particle Diameter (Draft Report dated May 12, 1997)	5/15/97
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II-I-31	Ltr/DOE-CAO/G. Dials to EPA/R. Trovato third response to EPA's letter of March 19, 1997 to DOE/A. Alm regarding CCA issues/comments. Supplemental information includes responses to Enclosures 1 of the March 19, 1997 letter as follows:	5/14/97
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Comment No. 1 - Origin of Hydrochemicals Facies and Model ed Paleof low Direct ions

Comment No. 4 - SECOTP2D - Test with a Heterogeneous T-Field

Comment No. 5 - SECOTP2D - Mass Balance

Comment No. 6 - Quantity Impacts of Code Errors

Comment No. 7 - SECOTP3D Code Test Results

Comment No. 8 - Benchmark NUTS with SWIFT

Comment No. 11 - Traceability of Development of Legacy Parameters

Comment No. 20 - Solution Mining

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Item No.	Title and/or Subject	Date of Document
II-I-33	Performance Assessment Parameter Values Identified in EPA letters to DOE dated April 17 and 25 1997	6/6/97
II-I-34	Ltr/DOE-CAO/G. Dials to EPA/L. Weinstock transmitting the final report on "Expert Elicitation on WIPP Waste Particle Size Distribution(s) During the 10,000-Year Regulatory Post-Closure Period" (Report filed A-93-02, II-G-24)	6/4/97
II-I-35	Ltr/DOE-CAO/J. Mewhinney to EPA/F. Marcinowski transmitting draft reports on "Results of the MgO Backfill Efficacy Investigation" (Filed A-93-02, Item II-A-39) and "Description and Evaluation of a Mechanistically Based Conceptual Model for Spall " (Filed A-93-02, Item II-G-23)	6/2/97
II-I-36	<p>Ltr/DOE-CAO/G. Dials to EPA/L. Weinstock responding to EPA's letter of March 19, 1997 requesting additional information regarding water flooding. This supplemental information includes the following:</p> <ul style="list-style-type: none"> a. Response to Enclosure 1, page 7, 40 CFR 194.32(e)-Scope of performance assessments b. Sandia National Laboratories - Waste Isolation Pilot Plant - Expedited CCA Activity - WPO #44158 Supplementary Analyses of the Effect of Salt Water Disposal and Waterflooding on the WIPP including: <ul style="list-style-type: none"> Atch 1: Injection Methods: Current Practices and Failure Rates in the Delaware Basin DOE/WIPP-97-2240, June 1997 Atch 2: Technical Review by Swift, et al of the HARTMAN Scenario: Implications for the WIPP by John Bredehoeft, June 13, 1997 	6/17/97
II-I-37	Ltr/EPA/L. Weinstock to DOE-CAO/G. Dials, providing follow-up information to concerns regarding performance assessment calculations identified in EPA's letter of March 19, 1997 to DOE/A. Alm with Enclosure entitled "Items Required for the EPA-Mandated Performance Assessment Verification Test" (4 pages).	7/2/97

- II-I-38 Ltr/DOE-CAO/G. Dials to EPA/L. Weinstock transmitting 7/25/97
intermediate results of the Performance Assessment
Verification Test (PAVT). **(This document is filed at A-
93-02, Item II-G-27)**
- V-B-5 Technical Support Document: Overview of Major
Performance Assessment Issues
- V-B-6 Technical Support Document for Section 194.23: Models
and Computer Codes
- V-B-7 Technical Support Document for Section 194.23: Ground
Water Flow and Contaminant Transport Modeling at WIPP
- V-B-8 Technical Support Document for Section 194.23: Potential
Effects of Mining on Ground Water Flow and Radionuclide
Transport at the WIPP Site
- V-B-9 Technical Support Document for Section 194.23: Density
Effects on Radionuclide Transport in the Culebra at the
WIPP Site
- 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-22 Technical Support Document for Section 194.32: Fluid
Injection Analysis