Recertification CARD No. 23
Models and Computer Codes

BACKGROUND (194.23(a))

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 the U.S. Department of Energy (DOE or Department) conducts peer review of conceptual models, as needed.

REQUIREMENT (194.23(a)(1))

(a) "Any compliance application shall include:

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

1998 CERTIFICATION DECISION (194.23(a)(1))

To meet the requirements for Section 194.23 (a)(1), the U.S. Environmental Protection Agency (EPA or Agency) expected DOE's application to contain a complete, clear, and logical description of each of the conceptual models used to demonstrate compliance. Documentation of the conceptual models was expected to 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 were to consider both natural and engineered barriers.

DOE's documentation of the conceptual model process and results was documented in Compliance Certification Application (CCA), Chapter 6 as well as in several appendices. In the original CCA PA DOE developed 24 conceptual models to describe the Waste Isolation Pilot Plant (WIPP) disposal system.

EPA determined that the CCA and supporting documentation contained a complete and accurate description of each of the conceptual models used and the scenario construction methods used. The scenario construction descriptions included sufficient detail to understand the basis for selecting some scenarios and rejecting others and were adequate for use in the CCA PA calculations. EPA found DOE in compliance with the requirements of Section 194.23 (a)(1).

A complete description of EPA's 1998 Certification Decision for Section 194.23(a)(1) can be obtained from Docket A-93-02, Items V-A-1 and V-B-2.

CHANGES IN THE CRA (194.23(a)(1))

For recertification, DOE undertook an extensive screening process to determine which Features, Events and Processes (FEPs) were still applicable to the disposal system and which changes were appropriate for the 2004 Compliance Recertification Application (2004 CRA) PA. As with the CCA, DOE developed scenarios to describe both undisturbed and disturbed performance (human intrusion) of the repository. DOE's 2004 CRA maintained 24 models to describe the WIPP disposal system. DOE did, however, modify three (3) conceptual models related to the Salado modeling: Disposal System Geometry, Repository Fluid Flow and the Disturbed Rock Zone (DRZ). DOE developed a new spallings model to replace the model found to be inadequate by the CCA Conceptual Peer Review Panel for the 2004 CRA PA.

Information on conceptual models and scenario construction is included in particular in 2004 CRA, Chapter 6, Sections 6.0.2.1, 6.0.2.2, 6.0.2.3, 6.2, 6.3, and 6.4; Appendix PA, Section PA-2.0; and Appendix PA, Attachment SCR. A number of 2004 CRA appendices and references provide specific information in support of Chapter 6 of the 2004 CRA, 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 (Docket A-93-02, Category II-G).

DOE's scenario construction methodology has not changed since the original CCA PA. Section 1.3.2.1 of the CCA CARD 23 discusses this process. DOE constructed two basic scenarios: undisturbed performance and disturbed performance, which includes drilling and mining events. As part of this scenario development DOE selected FEPs that were relevant. FEPs screened-in were included in the 24 conceptual models in the original CCA and has not changed in the 2004 CRA PA development.

The 24 conceptual models included in the CCA and the 2004 CRA are listed in Table 23-1 below, the four changed models are noted in bold type. 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 23-1 WIPP Conceptual Models Used in CCA and CRA PAs

	Conceptual 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.

BOLD - Modified and Peer Reviewed in 2004 CRA PA

EVALUATION OF COMPLIANCE FOR RECERTIFICATION (194.23(a)(1))

EPA's 2004 CRA review of compliance with 40 CFR 194.23 (a)(1) focused on any changes to FEPs, conceptual models, scenarios, or models since the 1998 Certification Decision. DOE's CCA and 2004 CRA scenario construction process has not changed and 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 2004 CRA, Chapter 6.2.1 and CCA, Chapter 6). DOE's methodology for addressing conceptual model development and scenario construction has also not changed since the original CCA and consisted primarily of identifying and screening processes and events and combining them into scenarios. EPA reviewed each of the steps that DOE used in this process during its evaluation and review of any changes since the original CCA.

During our 2004 CRA review, EPA found the information documenting DOE's FEPs reevaluation process to be generally thorough and complete (see also 2004 CRA CARD 32—Scope of Performance Assessments, for a more complete discussion of FEPs at the WIPP site). In 2004 CRA, Appendix PA, Attachment SCR-1.0, DOE summarized the results of the 2004 CRA FEPs reevaluation. Of the original 237 CCA FEPs, 106 have not changed in the 2004 CRA, and 120 FEPs required minor updates to their FEP descriptions and/or screening arguments. Seven of the original baseline FEPs screening decisions were changed, four FEPs have been deleted or combined with other related FEPs, and two new FEPs have been added to the list (See Table 23-2, below, for a summary of these changes). EPA reviewed DOE's FEP reevaluation and found their documentation to be adequate and their reasons for changes to the FEPs list reasonable.

Table 23-2 FEPs Change Summary Since CCA in 2004 CRA

EPA FEP I.D.	FEP Name	Summary of Change
		FEPs Combined with other FEPs
N17	**Lateral Dissolution**	Combined with N16, **Shallow Dissolution**. N17 removed from baseline.
N19	**Solution Chimneys**	Combined with N20, **Breccia Pipes**, N19 removed from baseline.
H33	**Flow Through Undetected Boreholes**	Combined with H31, **Natural Borehole Fluid Flow**. H33 removed from baseline.
W38	**Investigation Boreholes**	Addressed in H31, **Natural Borehole Fluid Flow**, and H33, **Flow Through Undetected Boreholes**. W38 removed from baseline.
		FEPs With changed Screening Decisions
W50	**Galvanic Coupling**	SO-P to SO-C
W68	**Organic Complexation**	SO-C to UP
W69	**Organic Ligands**	SO-C to UP
H27	**Liquid Waste Disposal**	SO-R to SO-C
H28	**Enhanced Oil and Gas Production**	SO-R to SO-C
H29	**Hydrocarbon Storage**	SO-R to SO-C
H41	**Surface Disruptions**	SO-C to UP (HCN)
		New FEPs for CRA
H58	**Solution Mining for Potash**	Separated from H13, **Potash Mining**
H59	**Solution Mining for Other Resources**	Separated from H13, **Potash Mining**

From 2004 CRA Appendix PA, Attachment SCR, Table SCR-1

During our 2004 CRA evaluation, EPA paid particular attention to any change to the FEPs concerning human intrusion scenarios related to mining and oil and gas drilling; such as fluid injection and air drilling. Our review is documented in the Technical Support Document (TSD) Sections 194.32 and 33: Compliance Recertification Application Re-evaluation of

Selected Human Intrusion Activities (Docket A-98-49, Item II-B1-10). As noted in our TSD some parameters were updated since the CCA, such as drilling rate and other drilling related values, as a result of continued activities in the Delaware Basin. None of these parameter changes had a detrimental impact on our compliance determination as exhibited by the results of the new performance assessment, the PABC, done by DOE (Docket A-98-49, Item II-B1-16).

Drilling practices, such as injection techniques and air drilling, and mining activities have not changed very much since the CCA. Therefore, EPA does not believe that our original conclusions during the CCA need to be modified for the 2004 CRA.

In the original CCA 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. However, the peer review panel ultimately found that the results from the spallings model were 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 spallings model overestimates releases by up to 10 times or more (Spallings Release Position Paper, Docket A-93-02 Item II-G-23). In EPA's August 2002 Guidance Letter (Docket A-98-49, Item II-B3-36), the Agency instructed DOE to develop a new spallings model for the recertification performance assessment. The new spallings model included three major elements: consideration of multiphase flow processes in the intrusion borehole, consideration of fluidization and transport of waste particulates from the intact waste mass to the intrusion borehole, and a numerical solution for the coupled mechanical and hydrological response of the waste as a porous medium (See 2004 CRA CARD 27 information on the peer review of this model). EPA found the spallings model peer review to be adequate and the new spallings model to be an improved alternative model to the original CCA model (see Docket A-98-49, Items II-B1-14 and II-B1-16).

For recertification, DOE modified the Disposal System Geometry, Repository Fluid Flow, and DRZ conceptual models. These models were changed to reflect new information on the Salado and to incorporate EPA's mandated Option D panel closure design requirements. To accommodate these conceptual changes in the Salado flow model, DOE modified the BRAGFLO computational grid and the computational grid for the direct brine release (DBR) version of BRAGFLO. This was done to include the Option D panel closure design requirements. DOE also simplified the shaft in the BRAGFLO grid, changed fluid flow paths, and changed the DRZ porosity from a constant value to a sampled range. These new conceptual models were peer reviewed in the 2002 to 2003 timeframe. The 2004 CRA CARD 27 summarizes our review of the Salado peer review; we found these conceptual model changes to be adequate. EPA also reviewed the technical basis of these conceptual model changes and found them to be appropriate and well documented. EPA determined that while these new models better reflect the knowledge of the disposal system, the changes had little impact on the results of the performance assessment (see Docket A-98-49, Items II-B1-13 and II-B1-16).

EPA's review found that the 2004 CRA and supplementary information contained a complete and accurate description of each of the conceptual models changes and that documentation of all conceptual models continues to adequately discuss site characteristics and processes active at the site. EPA determined that the conceptual models continue to 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 continue to adequately describe the future characteristics of the disposal system and its environs. The conceptual models continue to reasonably describe the expected performance of the disposal system and incorporate reasonable simplifying assumptions of the behavior of the disposal system. EPA found that the modifications to four of the conceptual models are reasonable and the related 2004 CRA documentation is complete.

EPA did not receive any public comments on DOE's continued compliance with the models and computer codes requirements of Section 194.23(a)(1).

RECERTIFICATION DECISION (194.23(a)(1))

EPA concludes that the 2004 CRA continues to contain 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. Based on a review and evaluation of the 2004 CRA and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2004-0025, Air Docket A-98-49), EPA determines that DOE continues to comply with the requirements for Section 194.23(a)(1).

REQUIREMENT (194.23(a)(2))

(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."

1998 CERTIFICATION DECISION (194.23(a)(2))

To meet the requirements of 194.23(a)(2), EPA expected the CCA to describe 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 did not need to be as detailed as the description of the models actually used in the 2004 CRA (and described under Section 194.23(a)(1)).

In the original CCA, DOE provided a description of plausible alternative conceptual models considered but not used in the PAs in the CCA and supplementary information (CCA

Chapters 2, 9, and CCA Appendix MASS). DOE also explained the reasons why these alternative models were not used to describe the performance of the repository.

EPA reviewed the material on alternative conceptual models and the comments made by the Conceptual Model Peer Review Panel on alternative models. The Peer Review Panel identified no substantive issues regarding alternative models.

A complete description of EPA's 1998 Certification Decision for Section 194.23(a)(2) can be obtained from Docket A-93-02, Items V-A-1 and V-B-2.

CHANGES IN THE CRA (194.23(a)(2))

DOE provided discussion of the conceptual models used to describe the WIPP's performance in 2004 CRA Chapter 2, Chapter 6.4, and Chapter 9.3.1. Additional information on alternative conceptual models was included in CCA Appendix MASS-2 to MASS-11, 2004 CRA Appendix PA, Attachment MASS, Section MASS-2.0 and CCA CARD 23-Models and Computer Codes, in particular Table 2.

The Conceptual Models Peer Review Panel consideration of alternative conceptual models is described in 2004 CRA, Appendix PEER1. 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 CCA Appendix MASS, other information is in 2004 CRA Appendix PA, Attachment MASS and Attachment SCR).

DOE's conceptual models and model development approach has changed little since the original CCA. As DOE stated at the time of the CCA, 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.

DOE changed four conceptual models since the CCA, DOE developed a new Spallings model for the 2004 CRA and made minor changes to three other models: Disposal System Geometry, Repository Fluid Flow, and DRZ models – these changes can be considered as alternative models as described by 40 CFR 194.23(a)(2). All of these models were peer reviewed as required by 40 CFR 194.27. The development of the new Spallings model was in response to the results of the CCA conceptual model peer review that rejected DOE's original model. The other three models were mainly changed to accommodate the EPA mandated Option D panel closure condition of the original 1998 Certification Decision.

EVALUATION OF COMPLIANCE FOR RECERTIFICATION (194.23(a)(2))

EPA reviewed the 2004 CRA documentation listed above and reevaluated the CCA documentation, in particular CCA CARD 23, Table 2. Little has changed since the CCA related to alternative models. Four of 24 conceptual models have changed; DOE developed a new Spallings model and made minor changes to the Disposal System Geometry, Repository Fluid Flow, and DRZ models. DOE did peer reviews of these models as required by 40 CFR 194.27. EPA reviewed all aspects of DOE's work related to alternative conceptual models to confirm that DOE continues to comply with the requirements of 40 CFR 194.23(a)(2). EPA considers these conceptual model changes to be other alternative models of the system. The peer review panels also agreed. A brief discussion of these peer reviews are noted below.

The Salado Flow Conceptual Model Peer Review was performed from April 2002 to March 2003, publishing its final report in May of 2003. This peer review evaluated changes to three of twenty four conceptual models: Disposal System Geometry, Repository Fluid Flow, and DRZ. The three conceptual models were changed because of new information gained after the original certification or changes to conceptual model assumptions mandated by EPA in the final CCA decision, such as the Option D panel closure condition of the original certification. Some of the changes were: modification of the computational grid to accommodate the new panel closure requirement, shaft simplification, changes in fluid flow paths, and changing to a constant porosity from the DRZ to a range of values for the halite and anhydrite layers (see the peer review report for details in Docket A-98-49, Item II-B1-13 and 2004 CRA CARD 27). EPA found this peer review to be adequate.

The Spallings Model Peer Review was performed from July 2003 to October 2003, publishing its final report in October of 2003. This model was changed because the original CCA conceptual model peer review found the CCA spallings model to be inadequate, and EPA expected DOE to develop a new spallings model before the first recertification in 2004. The new spallings model includes three major elements: consideration of multiphase flow processes in the intrusion borehole, consideration of fluidization and transport of waste particulates from the intact waste mass to the borehole, and a numerical solution for the coupled mechanical and hydrological response of the waste as a porous medium. DOE developed a new numerical code, called DRSPALL, to implement the new spallings conceptual model that calculates the volume of WIPP solid waste that may undergo material failure and be transported to the surface as a result of a drilling intrusion. EPA reviewed the new Spallings Model Peer Review (Docket A-98-49, Item II-B1-14) and found it to be adequate (see 2004 CRA CARD 27 for more detail).

As part of EPA's alternative model review, EPA examined 2004 CRA documentation to determine if any other models had changed or if any new alternative models have been developed since the original CCA. EPA also reexamined the CCA, in particular CCA CARD 23, Table 2 to determine if any of DOE's original approach or justification has changed since the original certification. Based on this review, EPA determines that all alternative models have been

appropriately considered by DOE and that DOE continues to be in compliance with the requirements of 40 CFR 194.23(a)(2).

The public suggested that karst formation and processes may be a possible alternative conceptual model for flow in the Rustler Formation. Karst may be thought of as voids in near-surface or subsurface rock created by brine flowing when rock is dissolved. Public comments state that karst developed interconnected "underground rivers" that may enhance the release of radioactive materials from the WIPP. Because of this comment EPA required DOE to do a thorough reexamination of all historical data, information, and reports, both those done by DOE and others, to determine if karst features or development had been missed during the more than of work done at WIPP (Docket A-98-49, Item II-B2-53) and EPA did a thorough reevaluation of karst and of our work done during the original CCA (Docket A-98-49, Item II-B1-15). Our reevaluation of historical evidence and recent work by DOE has not shown even the remotest possibility of 'underground river" near WIPP nor has it changed our original CCA conclusions. Therefore, EPA believes karst is not a viable alternative model at WIPP. For a more complete discussion of EPA's reevaluation of Karst see CRA CARD 15 and Docket A-98-49, Item II-B1-15.

RECERTIFICATION DECISION (194.23(a)(2))

Based on a review and evaluation of the 2004 CRA and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2004-0025, Air Docket A-98-49), EPA determines that DOE continues to comply with the requirements for Section 194.23(a)(2).

REQUIREMENT (194.23(a)(3))

(a) "Any compliance application shall include:

(3) Documentation that:

(i) Conceptual models and scenarios reasonably represent possible future states of the disposal system.
(ii) Mathematical models incorporate equations and boundary conditions which reasonably represent the mathematical formulation of the conceptual models.

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

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

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

1998 CERTIFICATION DECISION (194.23(a)(3))

In the original CCA, DOE convened a Conceptual Models Peer Review Panel to review the 24 conceptual models used in the PA. The Peer Review Panel found all the conceptual models to reasonably represent possible future states of the repository and to adequate for use in the performance assessment except for the spallings conceptual model. EPA determined that the spallings model produced reasonable and conservative results and that all other conceptual models were adequate and found DOE in compliance with the requirements of Section 194.23(a)(3)(i).

During the original CCA, EPA performed an independent review of the computer codes that 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); whether the numerical models provide numerical schemes that enable the mathematical models to obtain stable solutions; the proper implementation into the computer codes, and finally confirmed the peer review process, as appropriate.

EPA reviewed the mathematical model equations and boundary conditions for the following codes: CUTTINGS_S, SECOTP2D, CCDFGF, PANEL, BRAGFLO, BRAGFLO as used for direct brine release calculations (DBR), NUTS, FMT and SANTOS. The codes that used numerical solvers include: SANTOS, CUTTINGS_S, SECOTP2D, PANEL, BRAGFLO, BRAGFLO as used for direct brine release (DBR) and NUTS. EPA performed an independent review of the PA computer codes used to support the CCA PA. EPA concluded that the mathematical models used to describe the conceptual models incorporated equations which reasonably represented the mathematical formulation of the conceptual models.

A complete description of EPA's 1998 Certification Decision for Section 194.23(a)(3) can be obtained from Docket A-93-02, Items V-A-1 and V-B-2.

CHANGES IN THE CRA (194.23(a)(3))

Conceptual Models Represent Possible Future States

Identical to the original certification, all conceptual models used in the WIPP PAs have been reviewed by conceptual model peer review panels. The peer review panels have considered whether a conceptual model represents possible future states of the disposal system. In each case the peer review panels have approved conceptual models considered; this was completed for the four conceptual models new or changed in the 2004 CRA.

Mathematical Models

In the 2004 CRA, DOE consolidated documentation of mathematical model equations, initial and boundary conditions primarily in 2004 CRA, Appendix PA-4.0 for the various codes. DOE also discussed specific topics in 2004 CRA, Appendix PA and Attachments PORSURF, MASS, SOTERM, and TFIELD. DOE documented each code's characteristics in the User's Manual and the other documents listed below (Docket A-98-49, Category II-B2):

♦ 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 Manual 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 continued to use these three additional documents as secondary references for the 2004 CRA PAs:

♦ Requirements Document & Verification and Validation Plan (RD/VVP)—a single document that identifies the computational requirements of the code (e.g., MODFLOW 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 re-creation of the code used in the CRA PAs. Using this information, the computer user can reconstruct the code or install it on an identical platform to that used in the CRA PAs. The document includes the source-code listing, the subroutine-call hierarchy, and code compilation information.

♦ 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, bench marking, and validation, and also documents results of the quality assurance procedures.

The mathematical equations or initial or boundary conditions for the following codes have not change since the original CCA: CUTTING_S, SANTOS, BRAGFLO, FMT, NUTS, PANEL and SECOTP2D. The text from the CCA CARD 23 is updated to provide continuity and to update references for the 2004 CRA documentation. Three new codes are included in this updated review: MODFLOW, PEST and DRSPALL.

Waste Area Computer Codes

As in the original CCA, 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 area portion of the repository in the 2004 CRA: 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 (2004 CRA Appendix PA-4.2.3). 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 (2004 CRA, Appendix PA-4.2). In addition to these mathematical models equations, the direct brine release calculations (DBR) use 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 (2004 CRA, Appendix PA-4.7). The results of the BRAGFLO and DBR calculations are then used by the NUTS and PANEL computer codes to calculate the transport of radionuclides.

FMT is a computer code that consists of mathematical models equations that predict actinide solubilities based on thermodynamics assumptions (2004 CRA, Appendix PA, Attachment SOTERM 3.3). The calculated actinide solubilities are used in NUTS and PANEL to calculate the actinide concentrations released from the repository

NUTS and PANEL use outputs from BRAGFLO, DBR, and FMT to calculate actinide concentrations released from the repository. NUTS is coupled with BRAGFLO and 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 of gas and brine velocities. NUTS uses mathematical model equations to scale the magnitude of the BRAGFLO releases using the actinide solubilities (2004 CRA Appendix PA-4.3). PANEL's mathematical model equations predict actinide solubilities as a function of oxidation state and radioactive decay and also predict actinide concentrations released (2004 CRA Appendix PA-4.4). 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 (2004 CRA, Appendix PA-4.2, PA-4.3, and PA-4.4).

Culebra Computer Codes

For the 2004 CRA, DOE changed the way Culebra transmissivities and flow calculations were calculated. Three computer codes were 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: PEST, MODFLOW, and SECOTP2D. The mathematical model equations that comprise the MODFLOW and PEST combination 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 (2004 CRA, Appendix PA, Attachment TFIELD-1.0).

The results of the PEST calculations are used to generate various transmissivities as input to the MODFLOW computer code used to calculate brine flow in the Culebra dolemite. The primary mathematical model equations incorporated into MODFLOW 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 (2004 CRA, Appendix PA-4.8). PEST is used to solve the problem of parameter estimation for any mathematical model and is coupled with MODFLOW to estimate a family of possible transmissivity fields to represent the possible range of uncertainty in these well data (2004 CRA, Appendix PA, Attachment TFIELD). SECOTP2D calculates the transport of contaminated waste through the Culebra dolomite and radioactive decay, dispersion, and molecular diffusion (2004 CRA, Appendix PA-4.9).

Drilling Related Computer Codes

In the 2004 CRA, two computer codes, CUTTINGS_S and DRSPALL, are 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 cavings4 and drill cuttings5 that occur if a borehole penetrates the waste (2004 CRA, Appendix PA-4.6). The mathematical model equations in DRSPALL also predict spallings releases6 if the upward pressure exceeds 8 MPa when the intrusion borehole penetrates the waste in the repository (2004 CRA, Appendix PA-4.6).

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

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

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

CCDFGF

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 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 (2004 CRA, Appendix PA-6.8).

Boundary Conditions

The following codes used in DOE's CRA PAs require initial and boundary conditions: SANTOS, BRAGFLO, DBR, MODFLOW, DRSPALL, and 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 MODFLOW (2004 CRA, Chapter 6, Figure 6-24).

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 2004 CRA, Appendix PA-4.3.4.

The computer code PANEL is used to estimate the transport of radionuclides from the repository to the Culebra for the E1E2 scenario only (i.e., interception of both the waste and a brine reservoir by a borehole); see CCA 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 (2004 CRA, Appendix PA-4.4.1). 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-term7 input and calculates the transport of actinides through the Culebra dolomite.

Models for solid release to the surface are also coupled to the BRAGFLO computer code calculations. The CUTTINGS_S and DRSPALL computer codes (cuttings, cavings, and spallings) use the results calculated by the BRAGFLO computer code. CUTTINGS_S and DRSPALL (2004 CRA Appendix PA-4.5 and PA-4.6) use fluid pressure, fluid saturation, and other necessary quantities from the BRAGFLO calculations to predict the solid waste released (2004 CRA Appendix PA-4.5). DOE developed a new spall model, DRSPALL, for the 2004 CRA PA. The new spall model includes a series of processes to model a spall release, these include: tensile failure of solid waste, fluidization of failed material, entrainment into the wellbore, and transport of waste material up the wellbore to the land surface. DRSPALL calculates failed waste releases using mathematical formulations and initial and boundary conditions documented in 2004 CRA, Appendix PA-4.6.2, PA-4.6.2.1.1, and PA-4.6.2.1.2. Results of DRSPALL are used in CUTTINGS_S to calculate the final spall release volumes (2004 CRA, Appendix PA-4.6).

The computer code BRAGFLO as used for direct brine release (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 (2004 CRA, Appendix PA-4.7.1). In other words, there is no interaction between drilling fluid and the overlying rock formations between the repository and the surface; the release is not retarded in the borehole. 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.

<u>Numerical Models</u>

Information used to evaluate the stability of numerical model numerical schemes was provided in the validation documents and Analysis Packages that DOE prepared for each of the 2004 CRA PA computer codes. As in the original CCA 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

[7] 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.

2004 CRA, Chapter 5.3.20.

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). Problems are generally documented in each code Analysis Package (Docket A-98-49, Category II-B2).

Computer Models

As in the original CCA, 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 2004 CRA, Chapter 5). The QAPs specify quality assurance requirements for each step of the software development process (see 2004 CRA 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 (2004 CRA, Chapter 5.3.20 and Appendix QAPD Section 6). 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, MODFLOW 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. SNL used the RD to document what the PA computer codes 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 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.

In the original CCA 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. DOE used the same process and requirements for the 2004 CRA PA computer codes.

EVALUATION OF COMPLIANCE FOR RECERTIFICATION (194.23(a)(3))

Conceptual Models

As in the original CCA, all conceptual models have been approved by conceptual model peer reviews that considered if conceptual models represent possible futures of the disposal system. EPA agrees with the peer review panels and therefore find that DOE continues to be in compliance with Section 194.23(a)(3)(i).

Mathematical Models

In the evaluation for recertification, EPA reevaluated each of the mathematical models for
the computer codes used in the 2004 CRA PAs 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 2004 CRA PAs. 2004 CRA, Appendix PA-4.0, User's Manual and Analysis Package for each code were the primary sources of information on the mathematical models employed in PA (Docket A-98-49, Category II-B2). In general, mathematical formulations were adequately explained and were reasonable. DOE adequately documented and described simplifications of

conceptual models in the 2004 CRA PAs. DOE provided an adequate technical basis to support the mathematical formulations.

Three codes required a full evaluation for the 2004 CRA PA. MODFLOW, PEST and DRSPALL are new to the PA and required a complete review. The other PA codes have not changed their mathematical model or initial and boundary conditions since the original CCA PA calculations. MODFLOW is a well known and well tested flow code. However, DOE fully tested MODFLOW to verify that it would perform adequately in the 2004 CRA PA calculations. EPA reviewed this testing to verify that MODFLOW was adequately test. EPA found that the mathematical and initial and boundary conditions applied to MODFLOW usage in the 2004 CRA PAs to be sufficiently documented and adequate (2004 CRA, Appendix PA-4.8). PEST is an acquired code used to solve the problem of parameter estimation for any mathematical model, but with specific application to WIPP PA for optimizing T-fields using pilot points in conjunction with the MODFLOW groundwater flow model. EPA reviewed the application of PEST to parameter estimation and found DOE's usage adequate (Docket A-98-49, Item II-B1-7). DRSPALL is a new program developed for the 2004 CRA PA calculations. In 2004 CRA Appendix PA-4.6, DOE provided a complete description of the mathematical model for the DRSPALL code. In 2004 CRA Appendix PA-4.6.2.1.1 and PA-4.6.2.1.2, DOE adequately described the initial and boundary condition for the DRSPALL code. (Docket A-98-49, Items II-B1-7, II-B1-8, and II-B1-16)

EPA also reevaluated 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 and that the codes have not changed since the original CCA PAs. EPA reviewed the testing of each code 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. EPA found that DOE continues to comply with Section 194.23(a)(3)(ii). (Docket A-98-49, Items II-B1-7, II-B1-8, and II-B1-16).

Numerical Models

EPA reviewed for the 2004 CRA all relevant documentation on numerical models solution schemes, which was primarily contained in 2004 CRA, Appendix PA, Analysis Packages, and supplementary information (e.g., User's Manuals, Validation Documents- Docket A-98-49, Category II-B2). EPA also reviewed the QA documentation packages for each code for completeness and technical adequacy.

For the 2004 CRA, EPA reviewed the testing used to qualify each code for use in the 2004 CRA PAs. EPA found that DOE had adequately set the range of functional tests for each code to verify that the code will perform as expected and provide reasonable results. (see each codes Verification and Validation document for details of this testing) EPA found that DOE continues to comply with the requirements of Section 194.23(a)(3)(iii) (Docket A-98-49, Items II-B1-7, II-B1-8, and II-B1-16).

Computer Models

EPA reviewed all of the relevant documentation pertaining to each of the major codes described above (i.e., DD, RD, VVP and VD) and 2004 CRA Appendix PA and the associated attachments. Since the original CCA EPA also periodically independently reviewed DOE's testing of each of these codes to verify that results appeared accurate and free of coding error (Docket A-98-49, Items II-B1-7, II-B1-8, and II-B1-16). EPA ultimately found that each performance assessment code produced results that show continued compliance with this requirement.

During its review, EPA questioned if SANTOS produced results that were an accurate implementation of the numerical models and was free of coding errors. Specifically, EPA questioned in completeness comments G-5-3 and G-8-2 (Docket A-98-48, Item II-B2-37) if SANTOS was properly tested for accuracy and if the average stress of less than 5 MPa SANTOS predicted for waste was reasonable. In DOE's response to EPA Comments G-5-3 and G-8-2, DOE showed that they performed a fully functionally test of SANTOS as part of their code qualification and DOE also compared the results of SANTOS calculations to SPECTRUM-32. The activities showed that SANTOS produces results that are adequate for the development of porosity surfaces used in the 2004 CRA PAs (Docket A-98-49, Item II-B1-17).

EPA was able to determine that the 2004 CRA PAs computer codes continue to comply with Section 194.23(a)(3)(iv).

Peer Review

DOE performed two peer reviews to support the 2004 CRA PA calculations. DOE developed a new Spallings model and made minor changes to the Disposal System Geometry, Repository Fluid Flow, and DRZ models.

The Salado Flow Conceptual Model Peer Review was performed from April 2002 to March 2003, publishing its final report in March 2003. This peer review evaluated changes to three of twenty four conceptual models: Disposal System Geometry, Repository Fluid Flow, and DRZ. EPA examined the peer review plan and the final peer review report for this peer review and found them to adequately fulfill the requirements of 194.27 and NUREG-1297. EPA also observed the actual performance of the peer review panel members, the selection of the panel, the interaction of the peer review panel with DOE and SNL, and the documents produced during and as a result of the peer review. EPA found the process comparable with requirements of 40 CFR 194.27 and the guidance in NUREG-1297 (Docket A-98-49, Item II-B1-13).

The Spallings Model Peer Review was performed from July 2003 to October 2003, publishing its final report in October of 2003. DOE developed this new model because the original conceptual peer review found the CCA spall model to be inadequate and EPA expected DOE to develop a new spall model before the first recertification in 2004. EPA examined the peer review plan and the final peer review report for this peer review and found them to adequately fulfill the requirements of 194.27 and NUREG-1297. EPA also observed the actual performance of the peer review panel, the selection of the panel members, the interaction of the panel with DOE and SNL, and the documents produced during and as a result of the peer review. EPA found the process done comparable with requirements of 40 CFR 194.27 and the guidance in NUREG-1297 (Docket A-98-49, Item II-B1-14).

EPA did not receive any public comments on DOE's continued compliance with the requirements of Section 194.23(a)(3).

RECERTIFICATION DECISION (194.23(a)(3))

Based on a review and evaluation of the 2004 CRA and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2004-0025, Air Docket A-98-49), EPA determines that DOE continues to comply with the requirements for Section 194.23(a)(3).

BACKGROUND (194.23(b))

Section 194.23(b) requires that computer codes be documented in accordance with a proper quality assurance methodology.

REQUIREMENT (194.23(b))

(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."

1998 CERTIFICATION DECISION (194.23(b))

To meet the requirements of Section 194.23(b), EPA expected the Compliance Certification Application (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 was expected to contain plan(s) for quality assurance software, software requirements documentation, software design and implementation documentation, software verification and validation documentation and user documentation. Based on EPA audits and CCA review, EPA found DOE in compliance with the requirements of Section 194.23(b).

A complete description of EPA's 1998 Certification Decision for Section 194. 23(b) can be obtained from Docket A-93-02, Items V-A-1 and V-B-2.

CHANGES IN THE CRA (194.23(b))

Chapter 5 of the 2004 CRA discusses DOE's quality assurance (QA) program. Discussion of software QA is provided in 2004 CRA, Chapter 5.3.20. The DOE's quality assurance program, dated May 2003, is contained in 2004 CRA Appendix QAPD. The DOE QAPD incorporates the requirements of ASME NQA-2a-1990 addenda, part 2.7, to ASME NQA-2-1989 edition, Section 6. See 2004 CRA 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.

EVALUATION OF COMPLIANCE FOR RECERTIFICATION (194.23(b))

EPA verified compliance with the requirements of Section 194.22(a)(2)(iv) by reviewing Section 6.0 of the CAO (Carlsbad Field Office) QAPD and conducting periodic inspections of the SNL and Westinghouse's Waste Isolation Division quality assurance programs since the original CCA decision. 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 found that DOE's quality assurance requirements for computer codes used in the PA and compliance assessment continue to be 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

EPA did not receive any public comments on DOE's continued compliance with the requirements of Section 194.23(b).

RECERTIFICATION DECISION (194.23(b))

Based on a review and evaluation of the 2004 CRA and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2004-0025, Air Docket A-98-49), EPA determines that DOE continues to comply with the requirements for Section 194.23(b).

BACKGROUND (194.23(c))

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 computer source codes.

REQUIREMENT (194.23(c))

(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."

> (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."
>
> (3) Detailed descriptions of the structure of the computer codes and complete listings of the source codes."
>
> (4) Detailed descriptions of data collection procedures, data reduction and analysis, and code input parameter development."
>
> (5) Any necessary licenses;
>
> (6) An explanation of the manner in which models and computer codes incorporate the effects of parameter correlation."

1998 CERTIFICATION DECISION (194.23(c))

EPA expected the CCA to provide 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 computer source codes (Docket A-93-02, Category II-G).

EPA's evaluation found that the CCA and supplementary information included an adequate description of each model used in the calculations; a description of 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; and reports of code verification, bench marking, validation, and QA procedures. EPA also found that DOE adequately provided a detailed description of the structure of the computer codes and supplied a complete listing of the computer source code in supplementary documentation to the CCA. The documentation of computer codes describes the structure of computer codes with sufficient detail to allow EPA to understand how software subroutines are linked. The code structure documentation shows how the codes operate to provide accurate solutions of the conceptual models. EPA found that DOE did not use any software requiring licenses.

EPA determined in the CCA that DOE, after additional work and improvement of records in the SNL Record Center, adequately provided a detailed listing of the code input parameters; listed sampled input parameters; provided a description of parameters and the codes in which they are used; discussed parameters important to releases; described data collection procedures, sources of data, data reduction and analysis; and described code input parameter development, including an explanation of QA activities. EPA determined that the CCA and supplementary information adequately discussed how the effects of parameter correlation are incorporated, explained the mathematical functions that describe these relationships, and described the potential impacts on the sampling of uncertain parameters. The CCA also adequately documented the effects of parameter correlation for both conceptual models and the formulation of computer codes, and appropriately incorporated these correlations in the PA.

A complete description of EPA's 1998 Certification Decision for Section 194.23(c) can be obtained from Docket, A-93-02, Items V-A-1 and V-B-2.

CHANGES IN THE CRA

194.23(c)(1)

The 2004 CRA documentation continues to adequately document the theoretical backgrounds and method of analysis. EPA also evaluated whether the 2004 CRA continued to contain documentation describing exactly how each of the codes was used to support the PA. The information that EPA reviewed for the 2004 CRA was primarily contained in User's Manuals, Validation Documents, Implementation Documents, and Requirements Document & Verification and Validation Plans for each code. The most relevant information related to these issues is found in the Users' Manuals and Analysis Packages for each code. The primary codes that EPA reviewed include: CUTTINGS_S, MODFLOW, SECOTP2D, SUMMARIZE, PRECCDFGF, CCDFGF, LHS, DRSPALL, PANEL, BRAGFLO, BRAGFLO as used for direct brine releases (DBR), NUTS, FMT, PEST, SANTOS and ALGEBRA (Docket A-98-49, Category II-B3).

See the Background section of CCA CARD 23 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 and CCA CARD 23 Sections 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. Most of the major codes used for modeling the PA in the 2004 CRA have not changed since the CCA PA calculations. Modeling the repository and its surroundings are CUTTINGS_S, SECOTP2D, CCDFGF, PANEL, BRAGFLO, BRAGFLO as used for direct brine releases (DBR), NUTS, FMT, and SANTOS (CRA Chapter 6.4.11). New codes added to the 2004 CRA PA since the CCA are MODFLOW, PEST, and DRSPALL. In addition, LHS and ALGEBRA perform critical functions of sampling of parameters and initializing data in order to run PA computer codes. Most of the 2004 CRA PA codes are documented in the following documents: User's Manual (UM), Analysis Packages (AP), Requirements Document & Verification and Validation Plan (RD/VVP), Validation Document (VD), Implementation Document (ID) (Changes in the 2004 CRA (see 194.23(a)(3) of this CARD for details).

In general, a set of these five documents exists for each of the codes. 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 2004 CRA (e.g., 2004 CRA, Appendix PA, and Appendix PA Attachment MASS and Attachment SOTERM). 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 (see 2004 CRA, Chapter 6 and Appendix PA).

194.23(c)(2)

As in the CCA, documentation for the 2004 CRA 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, MODFLOW, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO as used for direct brine release (DBR), NUTS, FMT, PEST, DRSPALL, SANTOS and ALGEBRA. Table 23-3 lists the requirements of 194.23(c)(2) and where these requirements are documented in DOE documents. EPA determined that DOE documents for the 2004 CRA continue to fulfill the requirements of 194.23(c)(2) after reevaluating these documents and evaluating the code verification, bench marking, and validation documentation.

Table 23-3 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	Implementation 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	□	□				□

	Document Containing Information					
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 CRA Appendix QAPD, Section 6.0.

194.23(c)(3)

The information relevant to compliance with Section 194.23(c)(3) was contained in the Implementation Document (ID) for each modeling code (see Docket A-98-49, Category II-B2). This document provided the information necessary for the recreation of the code as used in the 2004 CRA 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 CRA PA calculations. The document includes the source-code listing, the subroutine-call hierarchy, and code compilation information (Docket A-98-49, Items II-B1-7 and II-B1-8).

194.23(c)(4)

The primary sources of parameter information are 2004 CRA, Chapter 6 (especially Tables 6-10 to 6-30), Appendix PA, Attachment PAR, and other appendices describing specific computer codes and parameter records in the SNL Record Center. Records in the SNL Record Center that EPA used to evaluate parameters for the 2004 CRA include:

♦ SNL Form NP 9-2-1 WIPP Parameter Entry Form (PEF): 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. The PEF replaced the Form 464 used in the CCA PA.

♦ Requestor Documents or Forms: Requestor documentation documents parameters that involve considerable data reduction and analysis by the SNL Principal Investigator or other technical personnel. The Requestor documentation is the second step of PA parameter development. Data reduction and analysis are usually explained at this step. The Requester documentation replaced the Principle Investigator Records Packages used during the CCA PA.

♦ 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. The Parameter Records Packages used in the CCA PAs are now included in the 2004 CRA PAs.

Documentation review for each parameter began with the Parameter Entry Form (PEF). The need for further documentation in the other three 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 was a value requiring experimental data for verification. Table 23-4 describes the types of information found in each of these four documents and possible paths in documenting parameter record information.

The original CCA contained approximately 1,600 parameters and the 2004 CRA contains approximately 1,700 parameters that 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 1,700 parameters used in the 2004 CRA PA calculations (Docket A-98-49, Item II-B1-6). All of the documents listed above are used to explain the full development of parameter values used as inputs to the PA calculations. Table 23-

4 indicates the documents that contain information required under Section 194.23(c)(4).

194.23(c)(5)

As in the CCA, no licenses from software vendors were required to operate the codes essential for the WIPP PA. Most 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. MODFLOW and PEST are public domain codes and are readily accessible.

194.23(c)(6)

User-specified parameter correlations for sampled parameters were introduced into the 2004 CRA 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 2004 CRA 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.

DOE implemented parameter correlations in the WIPP PA using the LHS computer code (2004 CRA, Appendix PA-5.4). Parameter correlations were defined for only a few sampled parameters (2004 CRA, Appendix PA, Attachment PAR-4.0). DOE used the same methodology in the 2004 CRA as in the CCA to incorporate parameter correlation. DOE inversely correlated rock compressibility and permeability and introduced induced correlation as described in 2004 CRA Appendix PA, Attachment PAR-4.0.

EVALUATION OF COMPLIANCE FOR RECERTIFICATION (194.23(c))

194.23(c)(1)

EPA found DOE's description of the theoretical background of each code to be adequately documented, generally in the User's Manual and Analysis Packages. 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 (Docket A-98-49, Category II-B2).

EPA reevaluated for the 2004 CRA review 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.

EPA reviewed all of the relevant documentation pertaining to the theoretical development and application of the models. For further discussion of EPA's review of documentation of conceptual models, alternative conceptual models, and the Conceptual Models Peer Review Panel, see the "Evaluation of Compliance for Recertification" discussions for the requirements of Section 194.23 (a)(1), (a)(2), and (a)(3) above in this CARD. The majority of the information was located in the User's Manuals and Analysis Packages for each code. For the 2004 CRA Pas, DOE's theoretical background for almost all of the codes has not changes since the original CCA decision, therefore, the review documented in CCA CARD 23 has not changed. Since the CCA, DOE has continued to test the PA codes to verify that they still performed as they did during the CCA PA. EPA has periodically reviewed and inspected these activities to verify that the PA codes continue to produce adequate results (Docket A-98-49, Items II-B1-7 and II-B1-8). In the 2004 CRA, DOE modified Appendix PA to include the theoretical background, mathematical development, and numerical development of the main PA codes and its use in the 2004 CRA PA analyses.

Subsequent to the execution of the original 2004 CRA PA, DOE discovered problems with the method of analysis for a number of input files and computer code errors related to the SUMMARIZE, PRECCDFGF, and CCDFGF sequence of calculations (Completeness Comments C-23-1R, C-23-10R, C-23-11, C-23-18, Other-1 discuss these errors in Docket A-98-49, Items II-B1-34, II-B1-39, and II-B1-40). EPA requested that DOE verify that these errors were corrected and that the codes passed the correct information to assure the analysis methods and assessments achieve correct results. DOE modified the codes, adjust the analysis process, and retested to confirm that the errors had been corrected. DOE also reran parts of the original 2004 CRA PA to assess the impact of these corrections (Completeness comments C-23-1R, C-23-10R, C-23-11, and C-23-18 in Docket A-98-49, Items II-B1-34, II-B1-39, and II-B1-40). EPA reviewed this work to confirm DOE results. EPA found that DOE had corrected these errors and verified that the code obtained the correct data to perform their analysis for the 2004 CRA PAs (Docket A-98-49, Item II-B1-16).

EPA found that DOE's level of documentation continues to be consistent with the adequate level of documentation produced during the original CCA review. DOE continued to be in compliance with Section 194.23(c)(1).

Section 194.23(c)(2)

EPA reviewed all of the relevant documentation pertaining to the requirements specified in Section 194.23(c)(2) for the following codes: CUTTINGS_S, MODFLOW, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO as used for direct brine release (DBR), NUTS, FMT, PEST, DRSPALL, SANTOS and ALGEBRA (see Docket A-98-49, Items II-B1-7, II-B1-8, and II-B1-16). DOE's 2004 CRA code 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.

DOE replaced the SECOFL2D flow code used in the CCA PA with the MODFLOW-2000 flow code. In completeness comment C-23-3 (Docket A-98-49, Item II-B2-34). EPA asked DOE to explain why MODFLOW-2000 was used to replace SECOFL2D. The primary reasons given for the change is that MODFLOW-2000 is well supported by a large user base and is continuing to be developed, SECOFL2D is not; MODFLOW is designed to operate on multiple computer platforms, SECOFL2D was designed to work on only the VAX/Alpha platforms; and the new pilot point estimation code, PEST, was designed to use only MODFLOW-2000. EPA reviewed DOE's response to C-23-3, 2004 CRA, Appendix PA, Attachment TFIELD and determined that MODFLOW-2000 is a reasonable replacement to SECOFL2D and that the MODFLOW/PEST transmissivity field estimate combination is a significant improvement over the SECOFL2D/GRASP-INV combination used in the CCA PA. (Docket A-98-49, Item II-B1-16) DOE continues to comply with Section 194.23(c)(2).

194.23(c)(3)

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, MODFLOW, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO as used for direct brine release (DBR), NUTS, FMT, PEST, SANTOS, DRSPALL, SUMMARIZE, 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 2004 CRA documentation of computer codes continues to adequately describe the structure of computer codes with sufficient detail to allow EPA to understand how software subroutines were linked and how to execute the 2004 CRA PAs. DOE continues to comply with Section 194.23(c)(3).

194.23(c)(4)

DOE discussed information supporting parameter development in the 2004 CRA and related documents. EPA reviewed 2004 CRA Chapter 6.0, CRA Appendix PA, Attachment PAR, and parameter records located in the Sandia National Laboratories (SNL) WIPP Record Center. The parameter records at SNL Record Center include WIPP Parameter Entry Forms (PEF) (NP 9-2-1), Requestor documents or forms, Data Records Packages (DRP), and Analysis Packages (AP). EPA reviewed parameter documentation and record packages for a sample of the approximately 1,700 parameters used as input values to the 2004 CRA PA calculations. EPA's review of WIPP PA parameters took place in three phases, in 2003 EPA reviewed the transfer of parameters from the CCA database to a new database system (Docket A-98-49, Item II-B3-69), next EPA reviewed the parameters changed from the parameter transfer to the 2004

CRA PA calculations (Docket A-98-49 Item II-B1-12), and finally EPA reviewed the parameter changes and documentation for values changed for the PABC calculations required by EPA to confirm the impact of code errors and parameter changes on the PA compliance results (Docket A-98-49, Item II-B1-6). EPA found mostly minor concerns at each phase of the review. However, ultimately DOE reasonably corrected each concern and EPA verified that parameters used in the CRA PAs were adequately developed, document, and traceable. EPA determined that DOE continues to comply with 40 CFR 194.23(c)(4)

EPA 2004 CRA Parameter Review

EPA, as in the CCA, performed a thorough review of the parameters and parameter development process for the 2004 CRA PAs. For the 2004 CRA PA parameter review EPA focused its review on parameters that have changed or are new since the original CCA PAs. EPA's review of the parameters and parameter development is described in detail (Docket A-98-49, Items II-B3-69, II-B1-12, and II-B1-6). EPA reviewed parameter packages for a sample of approximately 1700 parameters used in the 2004 CRA PA calculations. Records reviewed include 2004 CRA Chapter 6, Tables 6-10 to 6-30 and Appendix PA Attachment PAR, WIPP Parameter Entry Forms (NP 9-2-1), Requestor documents, Analysis Packages (AP), and Data Records Packages (DRP).

DOE made a number of changes related to parameters that required EPA's review since the original CCA PA. In 2002 and 2003, DOE moved the parameter data used in the PA codes to new database software, a new operating system, and a new computer processor. DOE also changed some of the parameter values in the database and moved the WIPP Records Center from Albuquerque to Carlsbad, New Mexico. Even though EPA found minor procedural concerns during this review, EPA found the data to be transferred to the database system to be adequate and accurate, that parameters changed or added had been done properly and was ultimately traceable, and that the PA codes could successfully access the new database without error. EPA documented its review of these activities (Docket A-98-49, Item II-B3-69).

As preparation for the 2004 CRA PA calculations, EPA initiated a review of the 2004 CRA PA parameters near the end of 2003 and the beginning of 2004. The review focused on parameters that have change or are new since the CCA PA calculations. Of the approximately 1,700 parameters in the WIPP parameter database, EPA found 128 new parameters and 203 changes to existing parameters. Many of the parameter changes were due to revisions of the waste inventory values in the PA calculations and new parameters values used in the new spall code, called DRSPALL. For most of the parameters changed and added EPA was able to verify that they were adequately recorded in the WIPP parameter database and that these parameters were justified and traceable to adequate supporting documentation.

During this review, EPA found that some WIPP 2004 CRA PA parameters where not recorded in the WIPP parameter database as expected. Parameters used in codes executed, such as MODFLOW, PEST, and SANTOS, on other computer platforms were not stored in the WIPP parameter database. EPA noted these as open issues in this report. EPA documented this review (Docket A-98-49, Item II-B1-12).

Subsequent to the early 2004 review, EPA continued to evaluate open issues related to parameters not recorded in the WIPP parameter database. This review documented closure to most of the issues found in EPA 2004 and verified that the 2004 CRA PA codes used parameters values extracted from the WIPP parameter database, the PAPDB. EPA found that some parameter values used in the 2004 CRA PA were set outside the parameter database, however in all cases DOE/SNL was able to provide adequate documentation justifying this approach. DOE was also able to reasonably document and justify parameters not in the parameter database used in the MODFLOW and PEST PA calculations. SNL used a special configuration management system (CMS) on the Alpha cluster of VAX computers for most of the 2004 CRA PA codes and the Linux Concurrent Versions System (CVS) file management systems at SNL for MODFLOW and PEST for example which contained all the codes and parameter data needed to run the PA (Docket A-98-49 Item II-B1-12). The CMS and CVS archives all the input files, output files, source code, and executable files of the modeling codes used by DOE in the PA modeling (Completeness Comments C-23-8 and C-23-9 in Docket A-98-49, Item II-B2-35). DOE was able to produce sufficient documentation to prove that these parameter values were supported by documentation and reasonably traceable – albeit difficult at times. This final WIPP 2004 CRA PA parameter report is documented (Docket A-98-49, Item II-B1-12).

EPA also reviewed parameter changes and issues related to the new 2004 CRA performance assessment baseline calculations, the PABC, mandated by EPA to establish a new PA baseline, to correct code and code execution errors, and to modify PA parameters EPA believed needed modification. This review is documented (Docket A-98-49, Item II-B1-6).

EPA's 2004 CRA PA parameter review addressed parameter identification, PA code parameter database access, and traceability of parameters used in the WIPP CRA PAs. The SNL practice of omitting some parameters used in the 2004 CRA PA from the PAPDB makes it difficult to identify all parameters used in the 2004 CRA PA and to trace the parameter information documentation that justified the values for all the parameters used in the 2004 CRA PA. Placing all parameters used in the PA calculations in the PAPDB or a centralized WIPP database would provide a more efficient means of identifying and reviewing parameters, thus facilitating traceability reviews. Alternative systems may be acceptable for some analyses if they can provide an equivalent level of parameter identification and supporting documentation as that present for the existing PAPDB. In addition, the practice of permitting data entry staff to make changes to the data entry forms may result in data entry errors or data values not intended by the data originator also complicated our review. Although current procedures do not explicitly prohibit this practice, the practice should be modified to ensure parameters are adequately documented and controlled.

During EPA's completeness review, stakeholders commented on the drilling rate used in the CRA PA calculations. During meetings with stakeholders in July of 2004, they complained about the drilling rate used in the CRA PA and suggested that a number two times the rate should be used in PA calculations. In a December 3, 2004, email EPA informed DOE that they were required to evaluate the impact of using twice the 2004 CRA PA drilling rate. DOE documented the results in DOE response to completeness comment Other-2 (Docket A-98-49, Item II-B2-39). EPA reviewed DOE's response and noted that doubling the drilling rate does increase predicted releases but that the results are still well within regulatory release limits.

Ultimately, EPA was able to determine that DOE continues to be in compliance with Section 194.23(c)(4).

Table 23-4 Location of Required Information on Parameters Used in Codes for Performance Assessment

□ = information meeting the requirement is found in this document

Requirement In Compliance Application Guidance	Document Containing Information								
	PEF[1]	PRP[2] Replaced by AP	PIRP[3]	DRP[4]	AP[5]	CRA, Vol. 1[6]	Att. PAR[7]	App. QAPD[8]	Parameter Database
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						□		□	

Table 23-4 Endnotes

[1] Sandia National Laboratories Form NP 9-2-1, WIPP Parameter Entry Form in SNL Records Center **[Replaced the Form 464 used in the CCA]**

[2] Parameter Records Packages in SNL Records Center **[Now located in Analysis Packages]**

[3] Principal Investigator Records Packages in SNL Records Center **[Now call the Requester]**

[4] Data Records Packages in SNL Records Center

[5] Analysis Packages

[6] See CRA Chapter 6 for parameter descriptions and Chapter 5 for an explanation of quality assurance activities

[7] CRA Appendix PA, Attachment PAR

[8] CRA Appendix QAPD

194.23(c)(5)

EPA's reevaluation focused on whether the 2004 CRA 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 2004 CRA PAs (Appendix PA-5.4 and Appendix PA, Attachment PAR-4.0). 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. EPA determined that DOE continues to comply with Section 194.23(c)(5).

194.23(c)(6)

EPA determined that parameter correlations were adequately explained in 2004 CRA Appendix PA, Attachment PAR-4.0 and were adequately incorporated. EPA also found that the 2004 CRA presented an adequate explanation of the manner in which models and computer codes incorporated the effects of parameter correlations. EPA determined that DOE continues to comply with Section 194.23(c)(6).

BACKGROUND (194.23(d))

The requirement expected DOE to provide EPA free access to PA models and computer code. DOE provided this access in both the CCA and 2004 CRA.

REQUIREMENT (194.23(d))

(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."

1998 CERTIFICATION DECISION (194.23(d))

During the review of the Compliance Certification Application (CCA), DOE provided EPA with ready access to computer hardware required to perform independent computer simulations. Therefore, EPA found DOE in compliance with the requirements of Section 194.23(d). See CCA CARD 23 for more information on EPA's 1998 Certification Decision.

A complete description of EPA's 1998 Certification Decision for Section 194.23(d) can be obtained from Docket A-93-02, Items V-A-1 and V-B-2.

CHANGES TO THE CRA (194.23(d))

No specific changes were made to the 2004 CRA to demonstrate compliance with Section 194.23(d).

EVALUATION OF COMPLIANCE FOR RECERTIFICATION (194.23(d))

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.

DOE provided 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 and the Linux Concurrent Versions System (CVS) file management systems at SNL which contained all the codes and parameter data needed to run the PA. The CMS and CVS archives all the input files, output files, source code, and executable files of the modeling codes used by DOE in the PA modeling (Completeness Comments C-23-8 and C-23-9 in Docket A-98-49, Item II-B2-35). DOE provided EPA and authorized personnel with unrestricted access to this computer hardware and software.

EPA did not receive any public comments on DOE's continued compliance with the requirements of Section 194.23(d).

RECERTIFICATION DECISION (194.23(d))

Based on a review and evaluation of the 2004 CRA and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2004-0025, Air Docket A-98-49) and adequate support and access to CRA PA computer codes, input files, and PA related documentation, EPA determines that DOE continues to comply with the requirements for Section 194.23(d).