**2009 Compliance Recertification Application (CRA-2009)**
**Compliance Application Review Document (CARD) No. 23**

# Models and Computer Codes

## 23.0 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 Department of Energy (DOE) conducts peer review of conceptual models, as needed.

## 23.1 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."

### 23.1.1 1998 CERTIFICATION DECISION (194.23(a)(1))

To meet the requirements for Section 194.23 (a)(1), EPA 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 Formation). The conceptual models were to consider both natural and engineered barriers.

DOE's conceptual model development and results were first documented in Compliance Certification Application (CCA) Chapter 6 as well as in several appendices. In the original CCA performance assessment (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 EPA Air Docket, A-93-02, Items V-A-1 and V-B-2.

### 23.1.2 CHANGES IN THE 2004 COMPLIANCE RECERTIFICATION APPLICATION (CRA-2004 OR CRA04) (194.23(a)(1))

For the 2004 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 (CRA-

2004 or CRA04) PA.  As with the CCA, DOE developed scenarios to describe both undisturbed and disturbed performance (human intrusion) of the repository.  DOE's CRA-2004 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 CRA-2004 PA.

Information on conceptual models and scenario construction was included, in particular in CRA-2004 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 Appendices PA, and  Feature, Event, and Process Screening for PA(SCR-2004).  A number of CRA-2004 appendices and references provide specific information in support of Chapter 6 of the CRA-2004, 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 did not change 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 did not change in the CRA-2004 PA development.

The 24 conceptual models included in the CCA and the CRA-2004 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 the CRA-2004 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 CRA-2004 PA

***BOLD-ITALIC*** **–** Modified and Peer Reviewed in CRA-2009 PABC

### 23.1.3 EVALUATION OF COMPLIANCE FOR 2004 RECERTIFICATION (194.23(a)(1))

EPA's CRA-2004 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 CRA-2004 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 CRA-2004 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 CRA-2004 review, EPA found the information documenting DOE's FEPs reevaluation process to be generally thorough and complete (see also CRA-2004 CARD 32—Scope of Performance Assessments, for a more complete discussion of FEPs at the WIPP site). In CRA-2004 Appendix PA, Attachment SCR-1.0, DOE summarized the results of the 2004 CRA FEPs reevaluation. Of the original 237 CCA FEPs, 106 had not changed in the CRA-2004, 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 had been deleted or combined with other related FEPs, and two new FEPs had been added to the list (See Table 23-2, below, for a summary of these changes in CRA-2004). 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 the 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 CRA-2004 Appendix PA, Attachment SCR, Table SCR-1

During our CRA-2004 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. EPA's review is documented in the CRA-2004 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, such as drilling rate and other drilling related values, were updated since the CCA 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 CRA-2004 PABC, done by DOE (Docket A-98-48 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 did not find that our original conclusions during the CCA needed to be modified for the CRA-2004.

During the original CCA, EPA reviewed each of the 24 conceptual models included 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 CCA peer review panel that all models except the spallings model were adequate for use in the PA calculations. However, the CCA 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 CCA PA spallings model overestimated 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 CRA-2004 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 CRA-2004 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 the 2004 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. CRA-2004 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 CRA-2004 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's conceptual models 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 were reasonable and the related CRA-2004 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).

### 23.1.4 2004 RECERTIFICATION DECISION (194.23(a)(1))

EPA concluded that the CRA-2004 continued to contain an adequate description of the scenario construction methods used, and that the scenario construction descriptions included sufficient detail to understand the basis for selecting some scenarios and rejecting others. Based on a review and evaluation of the CRA-2004 and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2004-0025, Air Docket A-98-49), EPA determined that DOE continued to comply with the requirements for Section 194.23(a)(1) for CRA-2004.

### 23.1.5 CHANGES IN THE 2009 COMPLIANCE RECERTIFICATION APPLICATION (CRA-2009 OR 2009 CRA) (194.23(a)(1))

For the 2009 recertification, as for the 2004 recertification, DOE undertook an extensive rescreening process to determine which FEPs were still applicable to the disposal system and which changes were appropriate for the 2009 Compliance Recertification Application (CRA-2009 or 2009 CRA) PA. This review is documented in CRA-2009 Appendix SCR-2009, Section SCR-1.0). Of the 235 FEPs considered for the CRA-2004, 189 remain the same, 35 have been updated with new information, 10 FEPs have been split into 20 similar but more descriptive FEPs, and one FEP has had its screening decision changed (See CRA-2009 CARD 32 for details of EPA's review of FEPs).

No changes in the 24 conceptual models or scenario construction methodology resulted from the FEPs reevaluation in the 2009 CRA (see Appendix SCR – 2009 and Appendix HYDRO-2009). However, because of new information, the Culebra Hydrogeology conceptual model was modified, peer reviewed (CRA-2009 CARD 27 and Burgess 2008), and used in the 2009 PABC (Kuhlman 2010b).

### 23.1.6 EVALUATION OF COMPLIANCE FOR 2009 RECERTIFICATION (194.23(a)(1))

EPA's CRA-2009 review of compliance with 40 CFR 194.23 (a)(1) focused on any changes to FEPs, conceptual models, scenarios, or models since the CRA-2004. During its CRA-2009 review, EPA found the information documenting DOE's FEPs reevaluation process to be generally thorough and complete (see also CRA-2009 CARD 32—Scope of Performance Assessments, for a more complete discussion of FEPs at the WIPP site). In CRA-2009 Appendix PA-2009, and CRA-2009 Appendix SCR-2009 SCR-1.0, DOE summarized the results of the CRA-2009 FEPs reevaluation. Of the original 235 CRA-2004 FEPs, 189 had not changed in the CRA-2009, and 35 FEPs required minor updates to their FEP descriptions and/or screening arguments. One of the original baseline FEPs screening decisions was changed, and ten FEPs were split into twenty FEPs to make them more descriptive. EPA reviewed DOE's FEP reevaluation and found its documentation to be adequate and its reasons for changes to FEPs reasonable.

EPA verified that no changes in the 24 conceptual models or scenario construction methodology resulted from the CRA-2009 FEPs reevaluation. DOE's scenario construction methodology has not changed since the CRA-2004 PA. The 24 conceptual models included in the CCA and the CRA-2004 have not changed for CRA-2009. These conceptual models are described in Section 23.1.2 and are listed in Table 23-1.

One conceptual model was changed for the 2009 PABC calculations because of new information derived from new monitoring wells and well testing activities. DOE modified the Culebra Hydrology Conceptual Model (in ***bold italics*** in Table 23-1) by making the model-derived transmissivity fields more geologically based. DOE's computational approach is basically the same as in the 2004 CRA, but the parameterization and some assumptions have been changed and refined based on new well data and testing, such as additional hydrochemical facies have been added based on new wells drilled (2009 CRA Appendix TFIELD-2009, Section TFIELD-1.0; Kuhlman 2010b Sections 2.0 and 3.0).

EPA examined DOE's conceptual model peer review (Burgess et al. 2008) and model changes implementation in developing the transmissivity fields (Kuhlman 2010b Section 3.0). The peer review panel for the original Culebra conceptual model found that the model was "inadequate" and "failed to correlate the detailed hydrogeology of the Culebra with its hydrologic character." In response to these concerns the Department conducted new studies and the findings are summarized as follows (Beauheim 2008, "Summary of Culebra Hydrology Conceptual Model and Numerical Implementation"):

- "A conceptual model has been formulated for the hydrology of the Culebra that integrates geologic, hydrologic, and geochemical data
- This model relates the flow properties of the Culebra to geologic factors that can be mapped with varying degrees of certainty over the model domain
- The model provides a statistical/stochastic basis for estimating hydrologic properties over the area of interest
- Geochemical observations are shown to be consistent with the conceptual model."

EPA's review of the technical work leading to the model revisions is described in CARD 15, Sections 15.2.4 and 15.2.5. EPA's oversight of the Revised Culebra Hydrology Conceptual Model Peer review is further discussed in Section 27.4.1 of CARD 27, Peer Review.

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) for CRA-2009.

### 23.1.7 2009 RECERTIFICATION DECISION (194.23(a)(1))

EPA concludes that the CRA-2009 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 CRA-2009 and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2009-0330, Air Docket A-98-49), EPA determines that DOE continues to comply with the requirements for Section 194.23(a)(1) for CRA-2009.

## 23.2 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."

### 23.2.1 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 CCA (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 EPA Air Docket, A-93-02, Items V-A-1 and V-B-2.

### 23.2.2 CHANGES IN THE 2004 COMPLIANCE RECERTIFICATION APPLICATION (CRA-2004 OR CRA04) (194.23(a)(2))

DOE provided discussions of the conceptual models used to describe the WIPP's performance in CRA-2004 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, CRA-2004 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 was described in CRA-2004 Appendix PEER.1. Although the FEP screening analysis was not intentionally designed to assist the development of alternative conceptual models, DOE used information generated during this process to support alternative conceptual model development (see CCA Appendix MASS, other information is in CRA-2004 Appendix PA, Attachment MASS and Attachment SCR).

DOE's conceptual models and model development approach have 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 between the CCA and CRA-2004. DOE developed a new Spallings model for the CRA-2004 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 changed mainly to accommodate the EPA mandated Option

D panel closure condition of the original 1998 Certification Decision.

### 23.2.3 Evaluation of Compliance for 2004 Recertification (194.23(a)(2))

EPA reviewed the CRA-2004 documentation listed above and reevaluated the CCA documentation, in particular CCA CARD 23, Table 2. Little changed between the CCA and CRA-2004 related to alternative models. Four of 24 conceptual models were changed in CRA-2004; DOE developed a new Spallings model and made minor changes to the Disposal System Geometry, Repository Fluid Flow, and DRZ models. DOE held 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's continued compliance with the requirements of 40 CFR 194.23(a)(2). EPA considers these conceptual model changes to be other alternative models of the disposal 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 CRA-2004 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 CRA-2004 CARD 27 for more detail).

As part of EPA's alternative model review, EPA examined CRA-2004 documentation to determine if any other models had changed or if any new alternative models had 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 had changed since the original certification. Based on this review EPA determined that all alternative models had been appropriately considered by DOE and that DOE continued 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 stated 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 perform a thorough reexamination of all historical data, information, and reports, produced by both DOE and others, to determine if karst features or development had been missed during the more than 30 years of work done at WIPP (Docket A-98-48 Item II-B2-53). EPA also did a thorough reevaluation of karst and of our work done during the original CCA (Docket A-98-46 Item II-B1-15). EPA's reevaluation of historical evidence and recent work by DOE indicated that there is no data supporting the possibility of an 'underground river" near WIPP, and confirmed our original CCA conclusions. Therefore, EPA found karst not to be a viable alternative model at WIPP. For a more complete discussion of EPA's reevaluation of Karst, see CRA-2004 CARD 15 and Docket A-98-49 Item II-B1-15.

### 23.2.4 2004 RECERTIFICATION DECISION (194.23(a)(2))

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

### 23.2.5 CHANGES IN THE 2009 COMPLIANCE RECERTIFICATION APPLICATION (CRA-2009 OR 2009 CRA) (194.23(a)(2))

One of the 24 conceptual models was changed since the CRA-2004. No other alternative conceptual models have been changed for the CRA-2009 PAs.

### 23.2.6 EVALUATION OF COMPLIANCE FOR 2009 RECERTIFICATION (194.23(a)(2))

EPA reviewed DOE's documentation; CRA-2009 Appendix PA-2009, Appendix SCR-2009, and Appendix MASS-2009; to verify that one conceptual model had been changed since CRA-2004 and that no new alternative conceptual models have been considered. In 2007 DOE considered modifying the cuttings and cavings and DRZ models. However, before the peer review process was completed, DOE decided to postpone these modifications (See CRA-2009 Section 27.7.3). EPA verified that these potential alternative conceptual models were never implemented in the CRA-2009 PAs.

The Culebra Hydrogeology Conceptual Model Peer Review was performed from August 11 to 14, 2008, publishing its final report in September 2008 [Burgess et al. 2008]. This peer review evaluated changes to the computational implementation and parameterization of the Culebra Hydrogeology Conceptual Model. 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 selection of the panel, the interaction of the peer review panel with DOE and SNL, the actual performance of the peer review panel members, and the documents produced during and as a result of the peer review. EPA found the process to comply with requirements of 40 CFR 194.27 and the guidance in NUREG-1297. [SCA 2008].

Once again, the public suggested that karst processes may be an alternative model (See the 2009 CARD Section 15.2.4 for EPA's review). Karst was considered and rejected as an alternate conceptual model by the Revised Culebra Hydrogeology Peer Review Panel (Burgess at al. 2008). EPA likewise thoroughly reviewed all available data and determined that karst processes are not active at the WIPP site and should not be included in the WIPP conceptual models.

### 23.2.7 2009 RECERTIFICATION DECISION (194.23(a)(2))

Based on a review and evaluation of the CRA-2009 and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2009-0330, Air Docket A-98-49), EPA determines that DOE continues to comply with the requirements for Section 194.23(a)(2) for CRA-2009.

## 23.3 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.

### 23.3.1 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 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 represented 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 EPA Air Docket, A-93-02, Items V-A-1 and V-B-2.

### 23.3.2 CHANGES IN THE 2004 COMPLIANCE RECERTIFICATION APPLICATION (CRA-2004 OR CRA04) (194.23(a)(3))

<u>Conceptual Models Represent Possible Future States</u>

As was the case during the original certification, all conceptual models used in the WIPP PAs had been reviewed by conceptual model peer review panels. The peer review panels considered whether a conceptual model represents possible future states of the disposal system. In each case, the peer review panels approved conceptual models considered. This process was completed for the four conceptual models new or changed in the CRA-2004.

<u>Mathematical Models</u>

In the CRA-2004, DOE consolidated documentation of mathematical model equations, initial and boundary conditions primarily in CRA-2004 Appendix PA-4.0 for the various codes. DOE also discussed specific topics in CRA-2004 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)—contains 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 CRA-2004 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 did not change between the original CCA and CRA-2004: CUTTING_S, SANTOS, BRAGFLO, FMT, NUTS, PANEL and SECOTP2D. The text from the CCA CARD 23 was updated to provide continuity and to update references for the CRA-2004 documentation. Three new codes were 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 CRA-2004: 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 (CRA-2004 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 (CRA-2004 Appendix PA-4.2). 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 (CRA-2004 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 (CRA-2004 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 (CRA-2004 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 (CRA-2004 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 (CRA-2004 Appendix PA-4.2, PA-4.3, and PA-4.4).

Culebra Computer Codes

For the CRA-2004, 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 (CRA-2004 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 dolomite. 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 (CRA-2004 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 (CRA-2004 Appendix PA, Attachment TFIELD). SECOTP2D calculates the transport of contaminated waste through the Culebra dolomite and radioactive decay, dispersion, and molecular diffusion (CRA-2004 Appendix PA-4.9).

Drilling Related Computer Codes

In the CRA-2004, two computer codes, CUTTINGS_S and DRSPALL, were 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 cavings[1] and drill cuttings[2] that occurs if a borehole penetrates the waste (CRA-2004 Appendix PA-4.6). The mathematical model equations in DRSPALL also predict spallings releases[3] if the upward pressure exceeds 8 MPa when the intrusion borehole penetrates the waste in the repository (CRA-2004 Appendix PA-4.6).

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 (CRA-2004 Appendix PA-6.8).

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

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

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

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 (CRA-2004 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 CRA-2004 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 (CRA-2004 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-term[4] 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 (CRA-2004 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 (CRA-2004 Appendix PA-4.5). DOE developed a new spall model, DRSPALL, for the CRA-2004 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 CRA-2004 Appendix PA-4.6.2, PA-4.6.2.1.1, and PA-4.6.2.1.2.

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4 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.

Results of DRSPALL are used in CUTTINGS_S to calculate the final spall release volumes (CRA-2004 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 (CRA-2004 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.

Numerical Models

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 CRA-2004 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 CRA-2004 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 is 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 were free of coding errors, SNL adopted a number of Quality Assurance Procedures (QAPs) (see CRA-2004 Chapter 5). The QAPs specify quality assurance requirements for each step of the software development process (see CRA-2004 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 (CRA-2004 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 CRA-2004 PA computer codes.

### 23.3.3 Evaluation of Compliance for 2004 Recertification (194.23(a)(3))

Conceptual Models

As in the original CCA, all conceptual models were approved by conceptual model peer reviews that considered if conceptual models represented possible futures of the disposal system. EPA agreed with the peer review panels, and therefore found that DOE continued to be in compliance with Section 194.23(a)(3)(i).

Mathematical Models

In the evaluation for the 2004 recertification, EPA reevaluated each of the mathematical models for the computer codes used in the CRA-2004 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 CRA-2004 PAs (see DOE's discussion CRA-2004 Appendix PA-4.0). The 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 CRA-2004 PAs. DOE provided an adequate technical basis to support the mathematical formulations.

Three codes required a full evaluation for the CRA-2004 PA. MODFLOW, PEST and DRSPALL were new to the PA and required a complete review. The other PA codes had 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 CRA-2004 PA calculations. EPA reviewed this testing to verify that MODFLOW was adequately tested. EPA found that the mathematical and initial and boundary conditions applied to MODFLOW usage in the CRA-2004 PAs to be sufficiently documented and adequate (CRA-2004 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 CRA-2004 PA calculations. In CRA-2004 Appendix PA-4.6, DOE provided a complete description of the mathematical model for the DRSPALL code. In CRA-2004 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 those 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 CRA-2004 all relevant documentation on numerical models solution schemes, which was primarily contained in CRA-2004 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 CRA-2004, EPA reviewed the testing used to qualify each code for use in the CRA-2004 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 continued 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 CRA-2004 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 it had performed a fully functional test of SANTOS as part of their code qualification, and compared the results of SANTOS calculations to SPECTRUM-32. These activities showed that SANTOS produced results that were adequate for the development of porosity surfaces used in the CRA-2004 PAs. (Docket A-98-49 Item II-B1-17)

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

Peer Review

DOE performed two peer reviews to support the CRA-2004 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 selection of the panel, the interaction of the peer review panel with DOE and SNL, the actual performance of the peer review panel members, 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 models and computer codes requirements of Section 194.23(a)(3).

### 23.3.4 2004 Recertification Decision (194.23(a)(3))

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

### 23.3.5 Changes in the 2009 Compliance Recertification Application (CRA-2009 or CRA09) (194.23(a)(3))

Specific details related to the Section 194.23(a)(3), as described above in Changes in the 2004 Compliance Recertification Application (194.23(a)(3)), have not changed and will not be repeated in the CRA-2009 discussion. See Sections 23.3.2 and 23.3.3**.**

<u>Conceptual Models Represent Possible Future States</u>

No changes were made to the conceptual models for the CRA-2009 PA and all conceptual models used in the CRA-2009 PA were previously peer reviewed. See CRA-2009 Section 23.3.5 for a discussion of modifications considered by DOE but not included in the CRA-2009 PA. DOE did change the implementation of conceptual model for the Culebra Hydrogeology Conceptual Model for the 2009 CRA PABC calculations, in particular the process used to calculate the Culebra transmissivity fields used in flow calculations. The original CCA peer review panel found the Culebra Hydrogeology Conceptual Model inadequate because a strong correlation was not established between the conceptual model and the numerical model used in performance assessment (SCA 2008 page 1). The objective of the new conceptual model for the 2009 PABC was to develop transmissivity fields for the Culebra that were: geologically based, consistent with observed ground water heads, consistent with groundwater responses in the Culebra pumping tests, and consistent with water chemistry results. The new Culebra Hydrology Conceptual Model was peer reviewed and approved (Burgess et al. 2008, Section 4.) for use in the performance.

<u>Mathematical Models</u>

The performance assessment mathematical models have not changed since the 2004 PABC calculations. The only changes were updates to parameters and the implementation of mathematical models using the new transmissivity field development process (Burgess etal. 2008, Kuhlman 2010b). DOE documented the various aspects of the mathematical models in numerous parts of the 2009 CRA, Appendix PA-2009 and Appendix MASS-2009. DOE documented mathematical model equations, initial and boundary conditions primarily in Appendix PA-2009 for the various codes. DOE also discussed specific topics in Appendices PA-2009, PORSURF-2009, MASS-2009, SOTERM-2009, and TFIELD-2009 and Clayton et al. (2009). DOE continued to document each code's characteristics in the User's Manual and Analysis Packages as described in Section 23.3.2 of this CARD. DOE also continued to use these additional documents: the Requirements Document & Verification and Validation Plan (RD/VVP), the Implementation Document (ID), and the Validation Document (VD) as secondary references for the CRA-2009 PAs codes.

Waste Area Computer Codes

Five computer codes continue to be used to solve mathematical model equations that incorporate a mathematical formulation of conceptual models of the future characteristics of the waste area of the repository: SANTOS, BRAGFLO, FMT, NUTS, and PANEL. The mathematical models for these codes have not changed since the 2004 CRA performance assessment calculations. The brief description of each code discussed in Section 23.3.2 of this CARD has not changed.

Culebra Computer Codes

Three computer codes continue to be 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 for the 2009 CRA PAs. The mathematical model equations that comprise the MODFLOW and PEST combination continue to be based on spatial correlations designed to predict the Culebra dolomite transmissivity fields (Kuhlman et al. 2010b). The computational approach described in Section 23.3.2 above - using PEST to solve the problem of parameter estimation, coupled to MODFLOW to estimate the family of possible transmissivity fields, and then using SECOTP2D to calculate transport of contaminated waste - has not changed in the 2009 CRA PAs. The changes to the transmissivity field derivation process have not changed the underlying conceptual models or mathematical formulations incorporated into the computer codes. The inclusion of more field pumping tests, additional pilot points, and including geologic effects represent an implementation change, rather than a conceptualization model change (Kuhlman et al. 2010b).

Drilling Related Computer Codes

CUTTINGS_S and DRSPALL continue to be 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 descriptions of these codes in Section 23.3.2 above have not changed in the 2009 CRA performance assessment.

CCDFGF

CCDFGF continues to be 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 continue to use 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.

Boundary Conditions

The following codes continue to require initial and boundary conditions: SANTOS, BRAGFLO, DBR, MODFLOW, DRSPALL, and SECOTP2D as described in Section 23.3.2 above. These initial and boundary condition requirements have not changed since the 2004 CRA PAs (EPA 2010b).

Numerical Models

Information used to evaluate the stability of numerical model numerical schemes continue to be provided in the validation documents and Analysis Packages that DOE prepared for each of the CRA-2004 PA computer codes as documented in Section 23.3.2 above (see DOE 2009 CRA Section 23.4.5.3 ). DOE's approach has not changed since the 2004 CRA.

Computer Models

DOE used the same computer code development process and requirements for the CRA-2009 PA computer codes as it has in the past, which consists of four primary development phases: 1) requirements phase, 2) design phase, 3) implementation phase and 4) software verification and validation. These are outlined in Section 23.3.3 above.

### 23.3.6 EVALUATION OF COMPLIANCE FOR 2009 RECERTIFICATION (194.23(a)(3))

Conceptual Models

As in the original CCA and 2004 CRA, all conceptual models have been approved by conceptual model peer reviews that considered whether conceptual models reasonably represent possible futures of the disposal system. EPA agrees with the peer review panels and therefore finds that DOE continues to be in compliance with Section 194.23(a)(3)(i).

Mathematical Models

The mathematical models used in the 2009 CRA PAs have not changed since the 2004 CRA. As in the evaluation for 2004 rectification, EPA reevaluated each of the mathematical models for the computer codes used in the CRA-2009 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 (EPA 2010e). The primary sources of information on the mathematical models employed in PA were CRA-2009 Appendix PA-2009, and User's Manual and Analysis Package (see a list of APs in 2009 CRA, Section 23, Table 23-4) for each code. Mathematical formulations continue to be adequately explained and were reasonable. DOE continues to adequately document and describe simplifications of conceptual models in the CRA-2009 PAs, and continues to provide an adequate technical basis to support the mathematical formulations (EPA 2010e).

EPA also reevaluated the functional tests for the 2009 CRA PA computer codes, described in the Validation Document for each computer code, to ensure that the codes have not changed and that DOE's tests of the computer code demonstrate that the code continues to perform as specified in the Requirements Document. 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 (see EPA 2010e). EPA found that DOE continues to comply with Section 194.23(a)(3)(ii) for the 2009 CRA. 16)

Numerical Models

EPA reviewed all relevant documentation on numerical model solution schemes, which continue to be primarily contained in CRA-2009 Appendix PA-2009, Analysis Packages, and supplementary information (e.g., User's Manuals, Validation Documents). EPA also reviewed the QA documentation packages for each code for completeness and technical adequacy. (EPA 2010e)

For the CRA-2009, EPA reviewed the testing used to qualify each code for use in the CRA-2009 PAs. EPA found that DOE continues to 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 code's 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).

Computer Models

EPA reviewed all of the relevant documentation pertaining to each of the major codes described above in Section 23.3.2 (i.e., DD, RD, VVP and VD) and 2009 CRA Appendix PA-2009 (EPA 2010e). EPA found that each performance assessment code produced results that show continued compliance with this requirement. EPA was able to determine that the CRA-2009 PAs computer codes continued to comply with Section 194.23(a)(3)(iv) (EPA 2010b).

Peer Review

DOE completed one peer review to support the CRA-2009 PABC calculations. DOE developed a new Culebra Hydrogeology Conceptual Model that was included in the 2009 PABC calculations.

The Culebra Hydrogeology Conceptual Model Peer Review was performed from August 11 to 14, 2008 publishing its final report in September 2008 (Burgess et al. 2008). This peer review evaluated changes to the computational implementation and parameterization of the Culebra Hydrogeology Conceptual Model. 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 selection of the panel, the interaction of the peer review panel with DOE and SNL, the actual performance of the peer review panel members, and the documents produced during and as a result of the peer review. EPA found the process to fulfill the requirements of 40 CFR 194.27 and the guidance in NUREG-1297 (SCA 2008). For further information, see CRA-2009 CARD 27, Peer Review.

EPA did not receive any public comments on DOE's continued compliance with the models and computer codes requirements of Section 194.23(a)(3) for CRA-2009.

#### 23.3.7 2009 RECERTIFICATION DECISION (194.23(a)(3))

Based on a review and evaluation of CRA-2009 and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2009-0330, Air Docket A-98-49), EPA determines that DOE continues to comply with the requirements for Section 194.23(a)(3) for the 2009 CRA.

## 23.4 BACKGROUND (194.23(b))

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

### 23.4.1 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 the ASME NQA-2a-1990 addenda, part 2.7, to ASME NQA-2-1989 edition."

### 23.4.2 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 EPA Air Docket, A-93-02, Items V-A-1 and V-B-2.

### 23.4.3 CHANGES IN THE 2004 COMPLIANCE RECERTIFICATION APPLICATION (CRA-2004 OR 2004 CRA) (194.23(b))

Chapter 5 of the CRA-2004 discusses DOE's quality assurance (QA) program. Discussion of software QA is provided in CRA-2004 Chapter 5.3.20. The DOE's quality assurance program, dated May 2003, is contained in CRA-2004 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 CRA-2004 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.

### 23.4.4 EVALUATION OF COMPLIANCE FOR 2004 RECERTIFICATION (194.23(b))

EPA verified compliance with the requirements of Section 194.22(a)(2)(iv) by reviewing Section 6.0 of the CBFO (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 CRA-2004 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 models and computer codes requirements of Section 194.23(b).

### 23.4.5 2004 RECERTIFICATION DECISION (194.23(b))

Based on a review and evaluation of the CRA-2004 and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2004-0225, Air Docket A-98-49), EPA determined that DOE continues to comply with the requirements for Section 194.23(b) for CRA-2004.

### 23.4.6 CHANGES IN THE 2009 COMPLIANCE RECERTIFICATION APPLICATION (CRA-2009 OR 2009 CRA) (194.23(b))

DOE's quality assurance program, dated November 2007, is contained in the 2009 CRA Appendix QAPD-2009. The DOE QAPD continues to incorporate the requirements of ASME NQA-2a-1990 addenda, part 2.7, to ASME NQA-2-1989 edition, Section 6. See CRA-2009 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.

### 23.4.7 EVALUATION OF COMPLIANCE FOR 2009 RECERTIFICATION (194.23(b))

DOE's computer code quality assurance program has not changed since the 2004 CRA. EPA verified that DOE continues to comply with the requirements of Section 194.22(a)(2)(iv) by reviewing Section 7.0 of the CBFO (Carlsbad Field Office) QAPD and conducting periodic inspections of SNL and Westinghouse's Waste Isolation Division quality assurance programs since the 2004 CRA CCA decision (2004 CRA Appendix QAPD-2009). 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 finds 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 is adequate. See CRA-2004 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 models and computer codes requirements of Section 194.23(b).

### 23.4.8 2009 Recertification Decision (194.23(b))

Based on a review and evaluation of the CRA-2009 and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2009-0330, Air Docket A-98-49), EPA determines that DOE continues to comply with the requirements for Section 194.23(b) for CRA-2009.

## 23.5 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.

### 23.5.1 Requirement (194.23(c))

(c) "Documentation of all models and computer codes included as part of any 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."

### 23.5.2 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 were incorporated, explained the mathematical functions that described 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 EPA Air Docket, A-93-02, Items V-A-1 and V-B-2.

### 23.5.3 Changes in the 2004 Compliance Recertification Application (CRA-2004 or 2004 CRA)

#### 23.5.3.1 194.23(c)(1)

The CRA-2004 documentation continued to adequately document the theoretical backgrounds and method of analysis. EPA also evaluated whether the CRA-2004 continued to contain documentation describing exactly how each of the codes was used to support the PA. The information that EPA reviewed for the CRA-2004 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 was found in the Users' Manuals and Analysis Packages for each code. The primary codes that EPA reviewed included: 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 CRA-2004 had not changed since the CCA PA calculations. Modeling the repository and its surroundings were CUTTINGS_S, SECOTP2D, CCDFGF, PANEL, BRAGFLO, BRAGFLO as used for direct brine releases (DBR), NUTS, FMT, and SANTOS (2004 CRA Chapter 6.4.11). New codes added to the CRA-2004 PA since the CCA were 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 CRA-2004 PA codes were 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) (see Section 23.3.2 in 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 CRA-2004 (e.g., CRA-2004 Appendix PA, and Appendix PA Attachment MASS and Attachment SOTERM). DOE's documentation also contained justification for the use of the models, the conceptual model derivation, the mathematical derivations, and the solution methods used in the codes (see CRA-2004 Chapter 6 and Appendix PA).

**23.5.3.2 194.23(c)(2)**

As in the CCA, documentation for the CRA-2004 regarding DOE's compliance with Section 194.23(c)(2) was 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 included: 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 CRA-2004 continued 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 2004 Performance Assessments**

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

= Information meeting the requirement is found in this document.

* = See 2004 CRA Appendix QAPD, Section 6.0.

#### 23.5.3.3 194.23(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 CRA-2004 PA calculations. With this information the user can compile the source code and install it on a computer system identical to that used in the CRA-2004 PA calculations. The document included the source-code listing, the subroutine-call hierarchy, and code compilation information. (Docket A-98-49 Items II-B1-7 and II-B1-8)

### 23.5.3.4 194.23(c)(4)

The primary sources of parameter information are CRA-2004 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 CRA-2004 include:

- SNL Form NP 9-2-1 WIPP Parameter Entry Form (PEF): All PA parameters were defined using this form, which contained the numerical values and distributions of parameters used as input to PA codes, identified the code the parameter is used in, and included 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 documented parameters that involve considerable data reduction and analysis by the SNL Principal Investigator or other technical personnel. The Requestor documentation was the second step of PA parameter development. Data reduction and analysis were 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 were typically generated for parameters that were 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 were 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 were 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 were included in the CRA-2004 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 CRA-2004 contained 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 were 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 described the methods that develop and support the approximately 1,700 parameters used in the CRA-2004 PA calculations (Docket A-98-49 Item II-B1-6). All of the documents listed above were 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).

**23.5.3.5 194.23(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.

**23.5.3.6 194.23(c)(6)**

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

### 23.5.4 Evaluation of Compliance for 2004 Recertification (194.23(c))

#### 23.5.4.1 194.23(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).

During the CRA-2004 review, EPA reevaluated 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 2004 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 CRA-2004 PAs, DOE's theoretical background for almost all of the codes had not changed since the original CCA decision; therefore, the review documented in CCA CARD 23 did not change. After the CCA, DOE had continued to test the PA codes to verify that they still performed as they did during the CCA PA. EPA periodically reviewed and inspected these activities to verify that the PA codes continued to produce adequate results (Docket A-98-49 Items II-B1-7 and II-B1-8). In the CRA-2004, DOE modified Appendix PA to include the theoretical background, mathematical development, and numerical development of the main PA codes and its use in the CRA-2004 PA analyses.

Subsequent to the execution of the original CRA-2004 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, adjusted the analysis process, and retested to confirm that the errors had been corrected. DOE also reran parts of the original CRA-2004 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's results. EPA found that DOE had corrected these errors and verified that the code obtained the correct data to perform their analysis for the CRA-2004 PAs (Docket A-98-49 Item II-B1-16).

EPA found that DOE's level of documentation continued to be adequate and consistent with the level of documentation produced during the original. DOE continued to be in compliance with Section 194.23(c)(1) for CRA-2004.

#### 23.5.4.2 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 CRA-2004 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 was that MODFLOW-2000 is well supported by a large user base and was continuing to be developed, SECOFL2D was not; MODFLOW was 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, CRA-2004 Appendix PA, Attachment TFIELD and determined that MODFLOW-2000 was a reasonable replacement to SECOFL2D and that the MODFLOW/PEST transmissivity field estimate combination was a significant improvement over the SECOFL2D/GRASP-INV combination used in the CCA PA. (Docket A-98-49 Item II-B1-16) DOE continued to comply with Section 194.23(c)(2).

#### 23.5.4.3 194.23(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 CRA-2004 documentation of computer codes continued 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 CRA-2004 PAs. DOE continued to comply with Section 194.23(c)(3) for CRA-2004.

#### 23.5.4.4 194.23(c)(4)

DOE discussed information supporting parameter development in the CRA-2004 and related documents. EPA reviewed CRA-2004 Chapter 6.0, CRA-2004 Appendix PA Attachment PAR, and parameter records located in the Sandia National Laboratories (SNL) WIPP Record Center. The parameter records at SNL Record Center included 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 CRA-2004 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 CRA-2004 PA calculations (Docket A-98-49 Item II-B1-12), and finally EPA reviewed the parameter changes and documentation for values changed for the CRA-2004 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. Ultimately DOE reasonably corrected each concern and EPA verified that parameters used in the CRA PAs were adequately developed, documented, and traceable. EPA determined that DOE continues to comply with 40 CFR 194.23(c)(4)

EPA CRA-2004 Parameter Review

EPA, as in the CCA, performed a thorough review of the parameters and parameter development process for the CRA-2004 PAs. For the CRA-2004 PA parameter review, EPA focused its review on parameters that had changed or were new since the original CCA PAs. EPA's review of the parameters and parameter development is described in detail in 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 CRA-2004 PA calculations. Records reviewed include CRA-2004 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 since the original CCA PA related to parameters that required EPA's review. 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 that the data transferred to the database system was adequate and accurate, that parameters changed or added had been done properly and were ultimately traceable, and that the PA codes could successfully access the new database without error. EPA documented its review of these activities in Docket A-98-49 Item II-B3-69.

In preparation for the CRA-2004 PA calculations, EPA initiated a review of the CRA-2004 PA parameters in late 2003 and early 2004. The review focused on parameters that had changed or were 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 parameter values used in the new spall code, 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 CRA-2004 PA parameters were not recorded in the WIPP parameter database as expected. Parameters used in codes executed on other computer platforms, such as MODFLOW, PEST, and SANTOS, were not stored in the WIPP parameter database. EPA noted these as open issues in this report and documented this review in 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 CRA-2004 PA codes used parameter values extracted from the WIPP parameter database, the PAPDB. EPA found that some parameter values used in the CRA-2004 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 that were 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 CRA-2004 PA codes, and the Linux Concurrent Versions System (CVS) file management systems at SNL for MODFLOW and PEST, for example. Together the CMS and CVS contained all the codes and parameter data needed to run the PA (Docket A-98-49 Item II-B1-12). The CMS and CVS archived 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 CRA-2004 PA parameter report was documented in Docket A-98-49, Item II-B1-12.

EPA also reviewed parameter changes and issues related to the new CRA-2004 performance assessment baseline calculations, the 2004 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 was documented in Docket A-98-49 Item II-B1-6.

EPA's CRA-2004 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 CRA-2004 PA from the PAPDB made it difficult to identify all parameters used in the CRA-2004 PA and to trace the parameter information documentation that justified the values for all the parameters used in the CRA-2004 PA. EPA recommended placing all parameters used in the PA calculations in the PAPDB or a centralized WIPP database as a more efficient means of identifying and reviewing parameters, thus facilitating traceability reviews. Alternative systems may be acceptable for some analyses if they provide an equivalent level of parameter identification and supporting documentation as that present for the existing PAPDB. In addition, EPA observed that permitting data entry staff to make changes to the data entry forms could result in data entry errors or data values not intended by the data originator. Current procedures did not explicitly prohibit this practice, which complicated EPA's ability to ensure that parameters are adequately documented and controlled.

During EPA's completeness review, stakeholders commented on the drilling rate used in the 2004 CRA PA calculations. During meetings in July of 2004, stakeholders objected to the drilling rate used in the 2004 CRA PA and suggested that a number two times the rate should be used in PA calculations. In a December 3, 2004, email, EPA requested that DOE evaluate the impact of doubling the CRA-2004 PA drilling rate. DOE documented the results in DOE's 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 increased predicted releases but that the results still fell within regulatory release limits.

Ultimately EPA was able to determine that DOE continued to be in compliance with Section 194.23(c)(4) for CRA-2004.

**Table 23-4 Location of Required Information on Parameters Used in Codes for 2004 Performance Assessments**

= 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 2004[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-2004 Chapter 6 for parameter descriptions and Chapter 5 for an explanation of quality assurance activities

[7] 2004-CRA Appendix PA, Attachment PAR

[8] 2004 CRA Appendix QAPD

### 23.5.4.5 194.23(c)(5)

EPA verified for CRA-2004, 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 required no license to execute or use. EPA confirmed that MODFLOW and PEST are public domain codes and are readily accessible. EPA determined that DOE continued to comply with Section 194.23(c)(5) for CRA-2004.

### 23.5.4.6 194.23(c)(6)

EPA's reevaluation focused on whether the CRA-2004 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 CRA-2004 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 manual, code section of EPA's 2004 computer code review technical support document (DOCKET NO: A-98-49, II-B1-7).

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

### 23.5.7 CHANGES IN THE 2009 COMPLIANCE RECERTIFICATION APPLICATION (CRA-2009 OR 2009 CRA)

### (194.23(c))

#### 23.5.7.1 194.23(c)(1)

The CRA-2009 documentation continues to adequately document the theoretical backgrounds and method of analysis. EPA evaluated whether the 2009 CRA continues to contain documentation describing exactly how each of the codes was used to support the PA. The information that EPA reviewed for the 2009 CRA continues to be primarily contained in UMs, VDs, IDs, and RD/VVPs for each code. The most relevant information continues to be found in the Users' Manual and Analysis Package for each code. The primary codes that EPA reviewed for the CRA-2009 included: CUTTINGS_S, MODFLOW, SECOTP2D, SUMMARIZE, PRECCDFGF, CCDFGF, LHS, DRSPALL, PANEL, BRAGFLO, BRAGFLO as used for direct brine releases (DBR), NUTS, FMT, PEST, SANTOS, ORIGEN2, and ALGEBRA.(EPA 2010e)

Information regarding whether the computer codes satisfied the requirements of Section 194.23(c)(1) is contained in the documents listed below for each modeling code. Most of the major codes used for modeling the PA in the 2009 CRA have not changed since the 2004 CRA PA calculations as described in Section 23.5.3.1 above. Modeling the repository and its surroundings were CUTTINGS_S, SECOTP2D, CCDFGF, PANEL, BRAGFLO, BRAGFLO as used for direct brine releases (DBR), NUTS, FMT, and SANTOS (2009 CRA Appendix PA-2009 Section PA-6.0). No new codes were added to the 2009 CRA PA. LHS and ALGEBRA continue to perform critical functions of sampling of parameters and initializing data in order to run PA computer codes. DOE continued to use the UM and AP documents to describe the conceptual models, mathematical models, and numerical methods that provide the basis for the theory and the assumptions underlying the PA codes. DOE included additional documentation in various appendices to the 2009 CRA (e.g., CRA-2009 Appendix PA-2009, Appendix MASS-2009, and Appendix SOTERM-2009). 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 (CRA-2009 Appendix PA-2009).

#### 23.5.7.2 194.23(c)(2)

Documentation for the CRA-2009 regarding DOE's compliance with Section 194.23(c)(2) continues to be primarily contained in UM, AP, VD, ID, and RD/VVP for each code. The codes that EPA reviewed included: CUTTINGS_S, MODFLOW, SECOTP2D, SUMMARIZE, PRECCDFGF, CCDFGF, LHS, PANEL, BRAGFLO, BRAGFLO as used for direct brine release (DBR), NUTS, FMT, PEST, DRSPALL, SANTOS,ORIGEN2, and ALGEBRA. Table 23-5 lists the requirements of 194.23(c)(2) and where these requirements are documented in DOE documents for CRA-2009. EPA determined that DOE documents for the CRA-2009 continue to fulfill the requirements of 194.23(c)(2) after reevaluating these documents and evaluating the code verification, bench marking, and validation documentation (EPA 2010e).

**Table 23-5 Location of Documentation for Models and Computer Codes Used in 2009 Performance Assessments**

| Requirement in Compliance Application Guidance | UM | AP | VD | ID | DD | RD/VVP | SNL QA Procedures* |
|---|---|---|---|---|---|---|---|
| General descriptions of the models | | | | | | | |
| Discussions of the limits of applicability of each model | | | | | | | |
| Detailed instructions for executing the computer codes | | | | | | | |
| Hardware requirements for executing the computer codes | | | | | | | |
| Software requirements for executing the computer codes | | | | | | | |
| Input and output formats with explanations of each input and output variable and parameter | | | | | | | |
| Listings of input and output files from a sample computer run | | | | | | | |
| Reports on code verification | | | | | | | |
| Reports on bench marking | | | | | | | |
| Reports on validation | | | | | | | |
| Reports on quality assurance procedures | | | | | | | |

= Information meeting the requirement is found in this document.

* = See 2009 CRA Appendix QAPD, Section 7.0.

**23.5.7.3 194.23(c)(3)**

The primary documentation of model compliance with Section 194.23(c)(3) continues to be contained in the Implementation Document (ID) for each modeling code. These code IDs provide the information necessary for the compiling of the codes as used in the CRA-2009 PA calculations. With this information the user can compile the source code and install it on a computer system identical to that used in the CRA-2009 PA calculations. The IDs continue to include the source-code listings, the subroutine-call hierarchies, and code compilation information.

**23.5.7.4 194.23(c)(4)**

The primary sources of parameter information are Fox (2008) for the CRA-2009, and Clayton (2010b) for the 2009 PABC, as well as 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 CRA-2009 include:

- ♦ SNL Form NP 9-2-1 WIPP Parameter Data Entry Form (PDE): All

PA parameters continue to be defined using this form, which contained the numerical values and distributions of parameters used as input to PA codes, identified the code the parameter is used in, and included information to trace the development of each parameter.

- ♦ Data Records Packages (DRP): These documents were typically generated for parameters that were 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 were 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 continue to be supplementary documents that generally describe all parameters used by a particular code in the PA calculations.

Documentation review for each parameter began with the Parameter Data Entry Form (PDE). 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 23-5 describes the types of information found in each of these four documents and possible paths in documenting parameter record information.

CRA-2009 Performance Assessment Parameter Database 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. CRA-2009 contains 90 new parameters and 16 changes to existing parameters (EPA 2010g, Table 1).

DOE uses the documents listed above to fully describe the methods used to develop and support the parameter values used as inputs to the CRA-2009 PA calculations. Table 23-6 indicates the documents that contain information required under Section 194.23(c)(4). Table 23-7 lists changes to the Performance Assessment since the 2004 PABC.

## Table 23-6 Location of Required Information on Parameters Used in Codes for 2009 Performance Assessments

= information meeting the requirement is found in this document

| Requirement In Compliance Application Guidance | PDE[1] | PIRP[2] | DRP[3] | AP[4] | Clayton 2010b or Fox 2008[5] | App. QAPD[6] | 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 23-6 Endnotes**

[1] Sandia National Laboratories Form NP 9-2-1, WIPP Parameter Data Entry Form in SNL Records Center

[2] Principal Investigator Records Packages in SNL Records Center

[3] Data Records Packages in SNL Records Center

[4] Analysis Packages

[5] Fox 2008 ERMS-549747 or Fox 2010b ERMS-552889 SNL

[6] 2009 CRA Appendix QAPD-2009

### 23.5.7.5 194.23(c)(5)

Licenses from software vendors are still not required to operate the codes essential for the WIPP PA. Most computer codes for the WIPP PA are developed by and programmed by SNL or its contractors as custom software, and require no license to execute. MODFLOW and PEST are public domain codes and are readily accessible.

### 23.5.7.6 194.23(c)(6)

User-specified parameter correlations for sampled parameters continue to be introduced into the CRA-2009 PA calculations using the Latin Hypercube Sampling (LHS) computer program. DOE continues to use 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 are explicitly correlated in the correlation matrix (or table) in the LHS computer code input file, which continues to be used in the CRA-2009 PA calculations (see Fox 2008, Section 4.0 for the 2009 CRA PA and Clayton 2010b, Section 4.0 for the 2009 PABC). For the 2009 CRA PAs, DOE also introduced a conditional relationship that was applied so that the sampled inundated rate is used as the maximum in the sampling for the humid rate. The DOE developed the LHSEDIT utility computer code to account for this conditional relationship (see Kirchner 2008b, page 135).

When values sampled using the LHS computer code are used to calculate other values, an induced correlation parameter relationship is created. This is the prevalent method of correlation used in the WIPP PA. DOE continues to use the same methodology in the CRA-2009 to incorporate parameter correlation. DOE inversely correlated rock compressibility and permeability and introduced induced correlation as described in Fox 2008 Section 4.0 for the 2009 CRA PA and Clayton 2010b Section 4.0 for the 2009 PABC.

**TABLE 23-7 CHANGES TO THE 2009 CRA PA**

| **2004 CRA PABC TO 2009 CRA PA CHANGES** | |
|---|---|
| Change | Documentation |
| DBR Parameters | Kirkes 2007 |
| CPR Degradation Rates | Kirchner 2008a |
| BRAGFLO Chemistry | Nemer and Clayton 2008 |
| Capillary Pressure and Relative Permeability Model | Nemer and Clayton 2008 |
| Drilling Rate | Clayton 2008b |
| Parameter Error Corrections; emplaced CPR error correction, halite/DRA parameters error correction, fraction of repository error correction, and NUTs and DBR calculations input files. | Nemer 2007b, Ismail 2007b, Dunagan 2007, Ismail 2007a, Clayton 2007 |
| | |
| **2009 CRA PA TO 2009 PABC CHANGES** | Clayton etal. 2009, Section 2. |
| Use 2008 PAIR inventory | Crawford etal. 2009, Fox 2009 |
| Use new T-fields | Burgess etal. 2008, Beauheim 2009 |
| Use most recent drilling rate, September 2008 | Clayton 2009a |
| Use most recent borehole plugging pattern probability, September 2008 | Clayton 2009a |
| Use new brine volume fir DBR calculations | Clayton 2009d |
| Use new mean solubilities for +III and +IV oxidation states | Brush etal. 2009, Xiong etal. 2009 |
| Correct panel volumes in BRAGFLO-DBR | Clayton 2009a |
| Matrix Partition Coefficients ($K_d$) | Clayton 2009e |

### 23.5.8 EVALUATION OF COMPLIANCE FOR 2009 RECERTIFICATION (194.23(c))

#### 23.5.8.1 194.23(c)(1)

In its 2009 CRA review, EPA found DOE's description of the theoretical background of each code to be adequately documented, particularly in each the User's Manual and the various 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 (see DOE 2009 CRA, Table 23.4 for a list of APs).

EPA reevaluated 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 (see EPA 2010e). Documentation was considered to continue to be complete if it contained sufficient information from which to judge whether the codes continued to be both formulated on a sound theoretical foundation and used properly in the 2009 CRA PA analyses.

EPA, for the 2009 CRA, reviewed all of the relevant documentation pertaining to the theoretical development and application of the models. The majority of the information was located in the User's Manuals and Analysis Packages for each code. For the CRA-2009 PAs, DOE's theoretical background for almost all of the codes has not changed. Therefore, EPA's reviews have not changed since the 2004 PABC. DOE continues to test the PA codes to verify that they still perform as they did previously (see EPA 2010e).

EPA found that DOE's level of documentation continues to be adequate and consistent with the level of documentation produced previously. DOE continues to be in compliance with Section 194.23(c)(1) for CRA-2009.

**23.5.8.2 194.23(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, ORIGEN2, and ALGEBRA (see EPA 2010e). DOE's CRA-2009 code documentation continues to provide 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 uses the same computer codes used in the 2009 CRA performance assessment calculations. DOE continues to comply with Section 194.23(c)(2) for CRA-2009.

**23.5.8.3 194.23(c)(3)**

During its 2009 CRA review, EPA examined 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, ORIGEN2, DRSPALL, SUMMARIZE, and ALGEBRA. EPA found that DOE submitted all of the source code listings. EPA continues to find the detailed descriptions of the structure of the computer codes to be adequate. The CRA-2009 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 CRA-2009 PAs. DOE continues to comply with Section 194.23(c)(3) for CRA-2009

**23.5.8.4 194.23(C)(4)**

DOE discussed information supporting parameter development in the 2009 CRA and related documents. EPA reviewed the 2009 CRA, DOE 2009 CRA Section 23, Fox 2008, Kirchner 2008a, and parameter records located in the Sandia National Laboratories (SNL) WIPP Record Center (see EPA 2010g). The parameter records at SNL Record Center included WIPP Parameter Data Entry Forms (PDE) (NP 9-2-1), 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 CRA-2009 PA calculations. EPA found one minor concern related to the hand-coding of parameters that are not included in the parameter database but are instead input manually: see Section 3.3 of the 2009 Parameter TSD (EPA 2010g). EPA recommended parameters that need to be included in the parameter database to improve traceability. DOE reasonably corrected this concern and EPA verified that parameters used in the 2009 CRA PAs were adequately developed, documented, and traceable. EPA determined that DOE continues to comply with 40 CFR 194.23(c)(4) for the 2009 CRA.

EPA CRA-2009 Parameter Review

EPA performed a thorough review of the parameters and parameter development process for the CRA-2009 PAs. For the CRA-2009 PA parameter review EPA continued to focus its review on parameters that have changed or were new since the previous recertification. EPA's review of the parameters and parameter development is described in detail in EPA's parameter TSD (EPA 2010g). EPA reviewed parameter packages for a sample of approximately 1700 parameters used in the CRA-2009 PA calculations. Documents reviewed include DOE CRA-2009 Section 23, Fox 2008 parameter tables, Kirchner 2008a, Clayton 2010b, WIPP Parameter Data Entry Forms (NP 9-2-1), Analysis Packages (AP), and Data Records Packages (DRP).

During this review, EPA found that some WIPP CRA-2009 PA parameters are still not recorded in the WIPP parameter database as expected: see EPA's parameter TSD Section 3.3 (EPA 2010g). EPA also reviewed parameter changes and issues related to the new CRA-2009 performance assessment baseline calculations (2009 PABC). The 2009 PABC was mandated by EPA to establish a new PA baseline using PA parameters which EPA believed needed modification, such as using the most recent inventory.

EPA's CRA-2009 PA parameter review continued to address parameter identification, PA code parameter database access, and traceability of parameters used in the WIPP 2009 CRA PAs, see EPA parameter review TSD (EPA 2010g). The SNL practice of continuing to omit some parameters used in the 2009 CRA PA from the PAPDB made it difficult to identify all parameters used in the CRA-2009 PAs and to trace the parameter information documentation that justifs the values for all the parameters used in the CRA-2009 PA calculations. Placing all the appropriate parameters used in the PA calculations in the PAPDB would provide a more efficient means of identifying and reviewing parameters, thus facilitating traceability reviews. This was also an issue in the 2004 CRA, see Section 23.5.4.4 above. In its October 19, 2009 completeness letter, item 3-23-10 EPA provided DOE a list of parameters EPA believed should be recorded in the parameter database. DOE responded by including these parameters in the database for the 2009 PABC calculations. EPA verified that these changes had been made to the parameter database (see EPA 2010g Section 5.0).

Ultimately, EPA was able to determine that DOE continues to be in compliance with Section 194.23(c)(4) for CRA-2009.

**23.5.8.5 194.23(c)(5)**

EPA verified that no licenses from software vendors are required to operate the codes essential for the WIPP PA for the 2009 CRA. EPA also verified that most computer codes for the WIPP PA were developed by and programmed by SNL or its contractors as custom software and requires no license. EPA confirmed that MODFLOW and PEST continue to be public domain codes and are readily accessible. EPA determined that DOE continued to comply with Section 194.23(c)(5) for CRA-2009.

#### 23.5.8.6 194.23(C)(6)

EPA verified that the 2009 CRA continues to contain 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 CRA-2009 PAs (Appendix PA-2009 Table PA-21, Fox 2008 Section 4.0; DOE 2009 CRA Section 23.11.5, and Clayton 2010b Section 4.0). EPA analyzed the computational aspects of the LHS computer program and functionality tests that implement the correlation check.

No changes were made in the parameter correlations sine CRA-2004 PABC, except the modification of conditional relationship between the inundated and humid microbial cellulose degradation rates. A conditional relationship was applied so that the sampled inundated rate is used as the maximum in the sampling for the humid rate, which improved the correlation (Kirchner 2008)

EPA determined that parameter correlations are adequately explained in CRA-2009 documents and are adequately incorporated in the 2009 PAs. EPA also found that the CRA-2009 presented an adequate explanation of the manner in which models and computer codes incorporated the effects of parameter correlations (Appendix PA-2009 Table PA-21). EPA determines that DOE continues to comply with Section 194.23(c)(6) for CRA-2009.

### 23.5.9 2009 RECERTIFICATION DECISION (194.23(c))

Based on EPA's review and evaluation of the 2009 CRA and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2009-0330, Air Docket A-98-49) determines that DOE continues to comply with the requirements for Section 194.23(c) for the 2009 CRA.

## 23.6 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 CRA.

### 23.6.1 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."

### 23.6.2 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 EPA Air Docket, A-93-02, Items V-A-1 and V-B-2.

### 23.6.3 Changes to the 2004 Compliance Recertification Application (CRA-2004 or CRA04) (194.23(d))

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

### 23.6.4 Evaluation of Compliance for 2004 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 models and computer codes requirements of Section 194.23(d).

### 23.6.5 2004 Recertification Decision (194.23(d))

Based on a review and evaluation of the CRA-2004 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-2004 PA computer codes, input files, and PA related documentation, EPA determined that DOE continued to comply with the requirements for Section 194.23(d) for CRA-2004.

### 23.6.6 Changes in the 2009 Compliance Recertification Application (CRA-2009 or CRA09) (194.23(d))

No specific changes were made to the 2009 CRA to demonstrate compliance with Section

194.23(d).

### 23.6.7 EVALUATION OF COMPLIANCE FOR 2009 RECERTIFICATION (194.23(d))

DOE continued 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 2009 CRA, and to assist EPA personnel in exercising DOE computer codes as needed.

DOE provided contacts at SNL and LANL 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 continues to use 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 contains all the codes and parameter data needed to run the PA. The CMS and CVS archive all the input files, output files, source code, and executable files of the modeling codes used by DOE in the PA. 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 models and computer codes requirements of Section 194.23(d).

### 23.6.8 2009 RECERTIFICATION DECISION (194.23(d))

Based on a review and evaluation of the 2009 CRA and supplemental information provided by DOE (FDMS Docket ID No. EPA-HQ-OAR-2009-0330, Air Docket A-98-49) and adequate support and access to CRA-2009 PA computer codes, input files, and PA related documentation, EPA determines that DOE continues to comply with the requirements for Section 194.23(d) for CRA-2009.