Title 40 CFR Part 191
Subparts B and C
Compliance Recertification Application
for the
Waste Isolation Pilot Plant

Models and Computer Codes
(40 CFR § 194.23)

United States Department of Energy
Waste Isolation Pilot Plant

Carlsbad Field Office
Carlsbad, New Mexico

Models and Computer Codes
(40 CFR § 194.23)

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Acronyms and Abbreviations

AP	Analysis Packages
ASME	American Society of Mechanical Engineers
CARD	Compliance Application Review Document
CCA	Compliance Certification Application
CRA	Compliance Recertification Application
DD	Design Document
DOE	U.S. Department of Energy
DRP	Data Records Packages
DRZ	Disturbed Rock Zone
EPA	U.S. Environmental Protection Agency
FEP	features, events, and process
IB	Inside Boundary
ID	Implementation Document
LHS	Latin Hypercube Sampling
NQA	Nuclear Quality Assurance
NRC	U.S. Nuclear Regulatory Commission
OB	Outside Boundary
PA	performance assessment
PABC	Performance Assessment Baseline Calculation
PEF	Parameter Entry Form
PIRP	Principal Investigator Records Package
QA	quality assurance
QAP	Quality Assurance Procedure
QAPD	Quality Assurance Program Document
RD	Requirements Document
SNL	Sandia National Laboratories
UM	User's Manual
VD	Validation Document
VVP	Verification and Validation Plan
WIPP	Waste Isolation Pilot Plant

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23.0 Models and Computer Codes (40 CFR § 194.23)

23.1 Requirements

§ 194.23 Models and Computer Codes

(a) Any compliance application shall include:

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

(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.

(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.

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

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

(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); listing 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.

(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.

23.2 40 CFR § 194.23(a)(1)

23.2.1 Background

The criteria in 40 CFR § 194.23(a)(1) (U.S. Environmental Protection Agency 1996) requires descriptions of the conceptual models and scenario construction used to demonstrate compliance.

23.2.2 1998 Certification Decision

To meet the requirements for section 194.23(a)(1), the U.S. Environmental Protection Agency (EPA) expected the U.S. Department of Energy (DOE) to include a complete, clear, and logical description of each conceptual model used to demonstrate compliance in the application. Documentation of the conceptual models was expected to discuss site characteristics and processes active at the site (e.g., gas generation or creep closure of the Salado salt formation). The conceptual models were to consider both natural and engineered barriers. The DOE developed 24 conceptual models to describe the Waste Isolation Pilot Plant (WIPP) disposal system.

For the Compliance Certification Application (CCA) (U.S. Department of Energy 1996), the EPA reviewed each of the 24 conceptual models included in the CCA (Table 23-1), using

Table 23-1. WIPP Conceptual Models

Conceptual Model	Component
1 Disposal System Geometry[a]	**Salado F/T**
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 DRZ	**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

[a] Entries in bold were modified and peer reviewed for the CRA-2004 PA.

information contained in the CCA, supplementary peer review panel reports, and supplementary information provided to the EPA by the DOE in response to specific EPA comments. Upon the conclusion of the conceptual model peer review, the panel states, "With the exception of the Spallings Model presented in the CCA, which the Panel continues to find inadequate, all remaining conceptual models have been determined to be adequate and all significant issues regarding their adequacy have been resolved" and "Although further refinement in understanding and predictive capability for spallings events would be desirable as part of a new conceptual model, the Panel has determined that the additional information presented by the DOE is sufficiently complete at this time to support a conclusion that the spallings volumes used in the CCA are reasonable, and may actually overestimate the actual waste volumes that would be expected to be released by the spallings process at the WIPP" (Compliance Recertification Application of 2004 [CRA-2004] [U.S. Department of Energy 2004], Appendix PEER-2004, Section PEER-2004 1.1.5, Section 4.0). The EPA agreed with the peer review panel that all models, with the exception of spallings, were considered adequate to represent future states of the repository. In the case of the spallings model, the EPA considered the results adequate, because the DOE showed in its additional spallings modeling that the release of solid waste predicted by the PA spallings model overestimated releases by a factor of 10 or more (Sandia National Laboratories and Carlsbad Area Office Technical Assistance Contractor 1997).

The EPA determined that the CCA and supporting documentation contained a complete and accurate description of each conceptual model and the scenario construction methods used in performance assessment (PA). 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. The EPA found the DOE to be in compliance with the requirements of section 194.23(a)(1) (Compliance Application Review Document [CARD] 23, Section 1.4 (U.S. Environmental Protection Agency 1998a).

A complete description of the EPA's 1998 Certification Decision for section 194.23(a)(1) can be obtained from CARD 23, Section 1.4 (U.S. Environmental Protection Agency 1998a).

23.2.3 Changes in the CRA-2004

For the CRA-2004, the 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 CRA-2004. The DOE's scenario construction methods have not changed since the CCA. The DOE constructed two basic scenarios: undisturbed performance and disturbed performance, which include drilling and mining events. As part of this scenario development, the DOE selected FEPs that were relevant. FEPs judged to be significant were included in the 24 conceptual models of the CCA and the CRA-2004.

The CCA FEPs were reassessed to determine if the screening justifications remained valid in light of changes within the WIPP project. Although minor changes were made to the FEPs, the results of the reassessment did not impact the original conceptual models or scenarios (CRA-2004, Appendix PA, Attachment SCR and Chapter 6.0, Section 6.2.6). In the CRA-2004, Appendix PA, Attachment SCR-1.0, the DOE summarized the results of the CRA-2004 FEPs reevaluation. Of the original 237 CCA FEPs, 106 had not changed in the CRA-2004, and 120 FEPs required minor updates to their descriptions and/or screening arguments (CRA-2004,

Appendix PA, Attachment SCR, Table SCR-2). The screening decisions for seven of the original baseline FEPs 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 for a summary of these changes).

Table 23-2. FEPs Change Summary in the CRA-2004[a]

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	Screened-out probability to screened-out consequence
W68	Organic Complexation	Screened-out consequence to undisturbed performance
W69	Organic Ligands	Screened-out consequence to undisturbed performance
H27	Liquid Waste Disposal	Screened-out regulatory to screened-out consequence
H28	Enhanced Oil and Gas Production	Screened-out regulatory to screened-out consequence
H29	Hydrocarbon Storage	Screened-out regulatory to screened-out consequence
H41	Surface Disruptions	Screened-out consequence to undisturbed performance
New FEPs for the CRA-2004		
H58	Solution Mining for Potash	Separated from H13, Potash Mining
H59	Solution Mining for Other Resources	Separated from H13, Potash Mining

[a] From the CRA-2004, Appendix PA, Attachment SCR, Table SCR-1.

The CRA-2004 maintained 24 conceptual models to describe the WIPP disposal systems. The DOE did, however, modify three conceptual models related to the Salado Formation modeling: Disposal System Geometry, Repository Fluid Flow, and the Disturbed Rock Zone (DRZ). Furthermore, the DOE developed a new spallings model for the CRA-2004. The 24 conceptual models included in the CCA and the CRA-2004 are listed in Table 23-1; the four changed models are noted in bold type. The components in this table refer to broad groupings of the conceptual models for those models related to human intrusion, flow and transport within the Salado Formation (Salado F/T), and flow and transport in hydrostratigraphic units other than the Salado (Non-Salado F/T).

23.2.4 EPA's Evaluation of Compliance for the 2004 Recertification

The EPA's review of the CRA-2004 for compliance with section 194.23(a)(1) focused on changes to FEPs, conceptual models, scenarios, or models since the 1998 Certification Decision (U.S. Environmental Protection Agency 1998b). The CCA and CRA-2004 scenario construction process had not changed and was based on screening decisions using a comprehensive list of FEPs developed for the Swedish Nuclear Power Inspectorate (also known as SKI), and other WIPP-specific FEPs developed by the DOE (see the CRA-2004, Chapter 6.0, Section 6.2.1, and the CCA, Chapter 6.0). The DOE's methods for addressing conceptual model development and scenario construction had not changed since the CCA, and consisted primarily of identifying and screening processes and events and combining them into scenarios. The EPA reviewed each of the steps used in this process during its evaluation and review of changes since the CCA. The EPA reviewed the DOE's FEPs reevaluation and found the documentation to be adequate and the reasons for changes to the FEPs reasonable (see Section 4.0 in U.S. Environmental Protection Agency 2006a).

During the CRA-2004 evaluation, the EPA paid particular attention to any FEP changes concerning human intrusion scenarios related to mining and oil and gas drilling, such as fluid injection and air drilling. The review is documented in *Technical Support Document for Sections 194.32 and 33: Compliance Recertification Application Re-evaluation of Selected Human Intrusion Activities* (U.S. Environmental Protection Agency 2006b). As noted in this document, 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. The parameter changes did not have a detrimental impact on the compliance determination, as exhibited by the results of the subsequent PA, the CRA-2004 Performance Assessment Baseline Calculation (PABC) (see U.S. Environmental Protection Agency 2006c, Section 11.3). Drilling practices, such as injection techniques and air drilling, and mining activities have not significantly changed since the CCA. Therefore, the EPA did not believe that the original conclusions during the CCA needed to be modified for the CRA-2004.

In the EPA's August 2002 Guidance Letter (Marcinowski 2002), the EPA instructed the DOE to develop a new spallings model for the CRA-2004 PA. The new spallings model (CRA-2004, Appendix PA, Attachment MASS-2004, Section 16.1.3) 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. The new spallings model was peer reviewed in 2003 and found to be adequate (CRA-2004, Chapter 9.0, Section 9.3.1.3.5 and CRA-2004, Appendix PEER-2004, Section PEER-2004 3.0). The EPA found the spallings model peer review to be adequate (U.S. Environmental Protection Agency 2006d, Section 5.0) and the new spallings model to be appropriate for use in the WIPP PA (see U.S. Environmental Protection Agency 2006c, Section 10.3.1).

The 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 the EPA-mandated Option D panel closure design requirements. The DOE modified the BRAGFLO computational grid and the computational grid for the direct brine release calculations to include the Option D panel closure design requirements. The DOE also simplified the shaft in the BRAGFLO grid and refined the BRAGFLO grid. These modified conceptual models were peer reviewed during 2002 to 2003 and found to be adequate (CRA-2004, Chapter 9.0, Section 9.3.1.3.4 and CRA-2004, Appendix PEER-2004, Section PEER-2004 2.0). The EPA found the Salado flow peer review to be adequate (see the U.S. Environmental Protection Agency 2006e, Section 5.0). The EPA determined that while these new models better reflected the knowledge of the disposal system, the changes had little impact on the results of the PA (U.S. Environmental Protection Agency 2006c, Section 12.0).

The EPA's review found that the CRA-2004 and supplementary information contained a complete and accurate description of each conceptual model that changed, and that documentation of all conceptual models continued to adequately discuss site characteristics and processes at the site. The EPA determined that the conceptual models continued to adequately represent those characteristics, processes, and attributes of the WIPP disposal system affecting its performance, and that the conceptual models considered both natural and engineered barriers. The EPA found that the DOE considered conceptual models that continued to adequately describe the future characteristics of the disposal system. The conceptual models continued to reasonably describe the expected performance of the disposal system and incorporate reasonable simplifying assumptions of the disposal system's behavior. The EPA found that the modifications to four of the conceptual models were reasonable and the related CRA-2004 documentation was complete (CARD 23, Section "Recertification Decision 194.23(a)(1);" U.S. Environmental Protection Agency 2006f).

The EPA concluded that the CRA-2004 continued 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-2004 and supplemental information provided by the DOE, the EPA determined that the DOE continued to comply with the requirements for section 194.23(a)(1) (CARD 23, Section "Recertification Decision 194.23(a)(1)," U.S. Environmental Protection Agency 2006f).

23.2.5 Changes or New Information Since the 2004 Recertification

A FEPs reassessment was conducted for the CRA-2009 and the results are documented in Appendix SCR-2009. In Appendix SCR-2009, Section SCR-1.0, the results of the CRA-2009 FEPs reevaluation are summarized. Of the 235 FEPs considered for the CRA-2004, 188 have not been changed, 35 have been updated with new information, 10 FEPs have been split into 20 similar but more descriptive FEPs, one screening argument has been changed to correct errors discovered during review, and one FEP has had its screening decision changed (Appendix SCR, Table SCR-2). Table 23-3 summarizes the FEPs that have been added, separated or had a screening decision change since the CRA-2004.

No changes in the 24 conceptual models or scenario construction methodology resulted from the FEPs reevaluation. Thus, the DOE continues to demonstrate compliance with the provision of section 194.23(a)(1).

Table 23-3. FEPs Change Summary Since CRA-2004[a]

EPA FEP I.D.[b,c]	FEP Name	Summary of Change
FEPs Clarified to be Less Generic		
H27	Liquid Waste Disposal – Outside Boundary (OB)	Name changed to "Liquid Waste Disposal Boundary – OB" to specify that this FEP pertains to those activities outside the WIPP land withdrawal boundary.
H28	Enhanced Oil and Gas Production – OB	Name changed to "Enhanced Oil and Gas Production – OB" to specify that this FEP pertains to those activities outside the WIPP land withdrawal boundary.
H29	Hydrocarbon Storage – OB	Name changed to "Hydrocarbon Storage – OB" to specify that this FEP pertains to those activities outside the WIPP land withdrawal boundary.
W6	Shaft Seal Geometry	Name changed to be specific to Shaft Seals, rather than generic "seals" which also included panel closures (seals).
W7	Shaft Seal Physical Properties	Name changed to be specific to Shaft Seals, rather than generic "seals" which also included panel closures (seals).
W8	Shaft Seal Chemical Composition	Name changed to be specific to Shaft Seals, rather than generic "seals" which also included panel closures (seals).
W17	Radiological Effects on Shaft Seals	Name changed to be specific to Shaft Seals, rather than generic "seals" which also included panel closures (seals).
W36	Consolidation of Shaft Seals	Name changed to be specific to Shaft Seals, rather than generic "seals" which also included panel closures (seals).
W37	Mechanical Degradation of Shaft Seals	Name changed to be specific to Shaft Seals, rather than generic "seals" which also included panel closures (seals).
W74	Chemical Degradation of Shaft Seals	Name changed to be specific to Shaft Seals, rather than generic "seals" which also included panel closures (seals).
FEPs With Changed Screening Decisions		
H41	Surface Disruptions	Screening changed from screened-out regulatory to screened-out consequence due to inconsistency with screening rationale.
New FEPs for CRA-2009		
H60	Liquid Waste Disposal – Inside Boundary (IB)	New FEP; separated from H27. The creation of this new FEP allows for more appropriate screening based on regulatory provisions pertaining to activities within the WIPP land withdrawal boundary.
H61	Enhanced Oil and Gas Production – IB	New FEP; separated from H28. The creation of this new FEP allows for more appropriate screening based on regulatory provisions that pertain to activities within the WIPP land withdrawal boundary.
H62	Hydrocarbon Storage – IB	New FEP; separated from H29. The creation of this new FEP allows for more appropriate screening based on regulatory provisions that pertain to activities within the WIPP land withdrawal boundary.
W109	Panel Closure Geometry	New FEP; separated from W6. The creation of this new FEP allows for more appropriate screening based on potential differences in design and composition of shaft seals versus panel closures.
W110	Panel Closure Physical Properties	New FEP; separated from W7. The creation of this new FEP allows for more appropriate screening based on potential differences in design and composition of shaft seals versus panel closures.

[a] From the Appendix SCR-2009, Table SCR-1.
[b] H = Human-induced FEP.
[c] W = Waste and Repository-Induced FEP.

Table 23-3. FEPs Change Summary Since CRA-2004[a] (Continued)

EPA FEP I.D.[b,c]	FEP Name	Summary of Change
W111	Panel Closure Chemical Composition	New FEP; separated from W8. The creation of this new FEP allows for more appropriate screening based on potential differences in design and composition of shaft seals versus panel closures.
W112	Radiological Effects on Panel Closures	New FEP; separated from W17. The creation of this new FEP allows for more appropriate screening based on potential differences in design and composition of shaft seals versus panel closures.
W113	Consolidation of Panel Closures	New FEP; separated from W36. The creation of this new FEP allows for more appropriate screening based on potential differences in design and composition of shaft seals versus panel closures.
W114	Mechanical Degradation of Panel Closures	New FEP; separated from W37. The creation of this new FEP allows for more appropriate screening based on potential differences in design and composition of shaft seals versus panel closures.
W115	Chemical Degradation of Panel Closures	New FEP; separated from W74. The creation of this new FEP allows for more appropriate screening based on potential differences in design and composition of shaft seals versus panel closures.

[a] From the Appendix SCR-2009, Table SCR-1.
[b] H = Human-induced FEP.
[c] W = Waste and Repository-Induced FEP.

23.3 40 CFR § 194.23(a)(2)

23.3.1 Background

40 CFR § 194.23(a)(2) requires a description of those conceptual models that were identified or developed while preparing the compliance application, but were determined not to be appropriate for portraying disposal system performance. It also requires that the reasons for not using these models be explained.

23.3.2 1998 Certification Decision

To meet the requirements of section 194.23(a)(2), the CCA described the plausible alternative conceptual models considered but not used and explained 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. In the CCA, the DOE describes plausible alternative conceptual models considered but not used for PA in the CCA and supplementary information (the CCA, Chapters 2.0, 9.0, and Appendix MASS). The DOE also explains why these alternative models are not used to describe the performance of the repository. The descriptions of the alternative models and justifications for the conceptual model selections are summarized in Dials (1997, Table 1). The EPA reviewed the material on alternative conceptual models and the comments made by the Conceptual Models Peer Review Panel on alternative models. The peer review panel identified no substantive issues regarding alternative models. The EPA found the DOE to be in compliance with the requirements of section 194.23(a)(2) (CARD 23, Section 2.4, U.S. Environmental Protection Agency 1998a).

A complete description of the EPA's 1998 Certification Decision for section 194.23(a)(2) can be obtained from CARD 23, Section 2.4 (U.S. Environmental Protection Agency 1998a).

23.3.3 Changes in the CRA-2004

As stated at the time of the CCA, the 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.

For the CRA-2004, the DOE describes the conceptual models used to evaluate the WIPP's performance in the CRA-2004, Chapter 2.0; Chapter 6.0, Section 6.4; and Chapter 9.0, Section 9.3.1. The DOE changed four conceptual models since the CCA. The DOE developed a new spallings model for the CRA-2004 and made minor changes to three other conceptual models: the Disposal System Geometry, Repository Fluid Flow, and DRZ models. These changes can be considered alternative models, as described by section 194.23(a)(2). All of these models were peer reviewed as required by 40 CFR § 194.27. The Conceptual Models Peer Review Panel's consideration of alternative conceptual models for the four changed conceptual models is described in the CRA-2004, Appendix PEER-2004, Sections PEER-2004 2.0 and PEER-2004 3.0.

23.3.4 EPA's Evaluation of Compliance for the 2004 Recertification

The EPA reviewed the CRA-2004 documentation listed above and reevaluated the CCA documentation. The EPA reviewed all aspects of the DOE's work related to alternative conceptual models to confirm that the DOE continued to comply with the requirements of section 194.23(a)(2) (CARD 23, Section "Evaluation of Compliance for Recertification 194.23(a)(2)," U.S. Environmental Protection Agency 2006f).

As part of the EPA's alternative model review, the EPA examined the CRA-2004 documentation to determine if any other models had changed or if any new alternative models had been developed since the CCA. The EPA also reexamined the CCA for alternative conceptual models seriously considered in the CCA, as summarized by Dials (1997, Table 1), to determine if any of the DOE's original approach or justification had changed since the original certification. Based on this review, the EPA determined that all alternative models had been appropriately considered by the DOE and that the DOE continued to be in compliance with the requirements of section 194.23(a)(2) (CARD 23, Section "Recertification Decision 194.23(a)(2)," U.S. Environmental Protection Agency 2006f).

Members of the public suggested that karst formation and processes may be a possible alternative conceptual model for flow in the Rustler. Karst may be thought of as voids in near-surface or subsurface rock created by water flowing when rock is dissolved. Public comments stated that karst could develop interconnected "underground rivers" that may enhance the release of radioactive materials from the WIPP. Because of this comment, the EPA required the DOE to perform a thorough reexamination of all historical data, information, and reports, both those by the DOE and others, to determine if karst features or development had been missed during previous work done at the WIPP. The DOE's findings are summarized in Lorenz (2006). The

EPA also conducted a thorough reevaluation of karst and of the work done during the CCA (U.S. Environmental Protection Agency 2006g). The reevaluation of historical evidence and recent work by the DOE did not show even the remotest possibility of an "underground river" near WIPP, nor did it change the CCA conclusions. Therefore, the EPA believed karst was not a viable alternative model at the WIPP. For a more complete discussion of the reevaluation of karst, see CARD 14/15 (U.S. Environmental Protection Agency 2006h) and Lorenz (2006).

Based on a review and evaluation of the CRA-2004 and supplemental information provided by the DOE, the EPA determined that the DOE continued to comply with the requirements of section 194.23(a)(2) (CARD 23, Section "Recertification Decision 194.23(a)(2)," U.S. Environmental Protection Agency 2006f).

23.3.5 Changes or New Information Since the 2004 Recertification

The 24 conceptual models have not changed since the CRA-2004 decision in March 2006. As part of DOE's continuous evaluation of alternative conceptual models, the DOE proposed in 2007 modifications that would affect two of the existing conceptual models, cuttings and cavings and DRZ (Vugrin and Nemer 2007). It was determined that since these proposed modifications would impact the conceptual models, an independent technical peer review on the adequacy of the proposed changes to the approved conceptual models should be performed in accordance with the requirements of section 194.27. Before the peer review was completed, the DOE decided in October 2007 to postpone the consideration of the proposed modifications (see Section 27.7.3). The DOE continues to demonstrate compliance with the provision of section 194.23(a)(2).

23.4 40 CFR § 194.23(a)(3)

23.4.1 Background

40 CFR § 194.23(a)(3) includes provisions to ensure documentation of the basis for conceptual models used in compliance applications. Specific requirements are for documentation that

1. Conceptual models and scenarios reasonably represent possible future states of the disposal system.

2. The equations and boundary conditions in a model reasonably represent the mathematical basis of the conceptual model.

3. Numerical schemes enable the mathematical models to obtain stable solutions.

4. Computer models implement the numerical models, have no coding errors, and produce stable solutions.

5. Peer review has been conducted on the conceptual models.

23.4.2 1998 Certification Decision

For the CCA, the DOE convened a Conceptual Models Peer Review Panel to review the 24 conceptual models used in PA (see Section 23.2.2). The EPA concurred with the panel's findings and found the DOE in compliance with the requirements of 40 CFR §§ 194.23(a)(3)(i) and 194.23(a)(3)(v).

During the CCA, the EPA performed an independent review of the computer codes, focusing on (1) 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); (2) whether the numerical models provided numerical schemes that enabled the mathematical models to obtain stable solutions; and (3) whether the computer codes were properly implemented.

The EPA independently reviewed the mathematical models and boundary conditions for the following codes: CUTTINGS_S, SECOFL2D, SECOTP2D, CCDFGF, PANEL, BRAGFLO, NUTS, FMT, SANTOS, and GRASP-INV. The codes that used numerical solvers included CUTTINGS_S, SECOFL2D, SECOTP2D, PANEL, BRAGFLO, NUTS, and SANTOS. The EPA concluded that the mathematical models incorporated equations that reasonably represented the conceptual models.

A complete description of the EPA's 1998 Certification Decision for section 194.23(a)(3) can be obtained from CARD 23, Sections 4.4, 5.4, 6.4, and 7.4 (U.S. Environmental Protection Agency 1998a).

23.4.3 Changes in the CRA-2004

23.4.3.1 Documentation

A description of the code documentation is given here for completeness and to aid in further discussion.

- 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 UM includes:
  - The numerical solution strategy and computational sequence, including program flowcharts and block diagrams.
  - The relationship between the numerical strategy and the mathematical strategy (e.g., 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 UM 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 UM 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 go beyond simple algebra (e.g., finite-difference, Simpson's rule, cubic splines, Newton-Raphson Methods, and Jacobian Methods). The UM explains the implementation of these methods in the computer code in sufficient detail that an independent reviewer can understand them.

- The derivation of the numerical procedure from the mathematical component model. The UM 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 UM 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 (APs)—contain detailed information on how the computer codes were used in the PA, including code implementation approaches and justification of parameters used. The DOE required each code to supply the following information relevant to 40 CFR § 194.23(c)(1) in its APs:
  - Description of the overall nature and purpose of the general analysis performed by the model. The APs describe the specific aspects of the analysis for which the model is used. The documentation shows input and output parameters of the model. The APs 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 APs 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.

The DOE continued to use five additional documents as secondary references for the CRA-2004:

- Requirements Document (RD)—identifies the computational requirements of the code (e.g., MODFLOW must be able to simulate groundwater flow under steady-state conditions)

- Verification and Validation Plan (VVP)—identifies tests and associated acceptance criteria for the code and validation that all aspects of the code work properly together.

- Design Document (DD)—describes the major features of the software design: the theoretical basis; the embodied mathematical model; control flow; control logic; data structures; functionalities and interfaces of objects; components, functions, and subroutines used in the software; and the allowed or prescribed ranges for data inputs and outputs in a manner that can be implemented.

- Implementation Document (ID)—provides the information necessary to recreate the code used in the PAs. Using this information, the computer user can reconstruct the code or install it on an identical platform to that used in the PAs. The document includes the source code listing, subroutine-call hierarchy, and code compilation information.

- Validation Document (VD)—summarizes the results of the testing activities prescribed in the RD/VVP documents for the individual codes and provides evaluations based on those results. The VD contains listings of sample input and output files from computer runs of each model. The VD also contains reports on code verification, bench marking, and validation, and documents the results of the quality assurance procedures (QAPs).

23.4.3.2 Conceptual Models

Analogous to the original certification, all modified conceptual models used in the WIPP PA were reviewed by conceptual model peer review panels. The peer review panels considered whether a conceptual model represents possible future states of the disposal system. For each of the four changed conceptual models in the CRA-2004 PA (see Section 23.2.3), the peer review panels approved the conceptual models considered (see CRA-2004, Appendix PEER-2004; Sections PEER-2004 2.0 and PEER-2004 3.0).

23.4.3.3 Mathematical Models

In the CRA-2004, the DOE consolidated computer code documentation of mathematical models and initial and boundary conditions, primarily in the CRA-2004, Appendix PA, Section PA-4.0. The DOE also discussed specific topics in CRA-2004, Appendix PA, and Attachments PORSURF, MASS, SOTERM, and TFIELD. The DOE documented each code's characteristics in the UM and the other documents listed in Section 23.4.3.1.

The mathematical models or initial or boundary conditions for the following codes did not change after the CCA: SANTOS, BRAGFLO, FMT, NUTS, PANEL, and SECOTP2D. The cuttings and cavings mathematical models in CUTTINGS_S were not changed, but the spallings mathematical models were replaced by the new DRSPALL code. Three new codes were included in the EPA's review for the CRA-2004: MODFLOW, PEST, and DRSPALL. See U.S. Environmental Protection Agency (2006i, 2006j) for more information on the code review conducted for the CRA-2004.

23.4.3.4 Numerical Models

Information used to evaluate the stability of the numerical schemes was provided in the VDs and APs that the DOE prepared for each of the CRA-2004 PA computer codes. The DOE's evaluation of numerical schemes to ensure the stability of the numerical solutions included an evaluation of the impact on previous analyses and any appropriate corrective actions to either the computer code or the earlier analyses. Errors that qualified as a condition adverse to quality, such as computer code stability problems, were controlled and resolved as described in the CRA-2004, Chapter 5.0, Section 5.3.20.

The DOE maintains a 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 and the number of numerical iterations required to reach convergence. Convergence criteria, and the maximum number of iterations allowed to achieve convergence, are set within various subroutines in the computer codes where appropriate. Although the DOE did not specify strict requirements for the convergence criteria, if the criteria are too lenient, the results will indicate potentially unstable solutions to the numerical model's numerical schemes. The code generates messages if the mathematical solution algorithm does not converge within the user-specified criteria (see the UM for each computer code). Problems are documented in each code's AP.

23.4.3.5 Computer Models

As in the CCA, to ensure that the DOE's computer codes accurately implement the numerical models and are free of coding errors, a number of QAPs were adopted (see the CRA-2004, Chapter 5.0). The QAPs specify quality assurance (QA) requirements for each step of the software development process (see CARD 22, U.S. Environmental Protection Agency 2006k, for a discussion of EPA's review of the DOE's QA program). This process involved four primary development phases: (1) requirements, (2) design, (3) implementation, and (4) verification and validation (CRA-2004, Chapter 5.0, Section 5.3.20 and Appendix QAPD, Section 6.0). The objective of each phase 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 to demonstrate that the computational requirements for the software are met. Two documents are produced during this phase: the RD and the VVP, which, when combined, are called RD/VVP. The RD contains the functional requirements that the proposed software must satisfy, with specific requirements relating to the aspects of the system to be simulated with a particular computer code. For example, groundwater flow through the Culebra Dolomite Member of the Rustler (hereafter referred to as 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 and associated acceptance criteria to ensure verification of each software development phase (i.e., that the portion of the code being tested matches known solutions) and validation of the entire software baseline the first time the computer code is placed under QA control (i.e., that all aspects of the code work together properly). The RD documents what the PA computer codes do by listing the functional requirements of each computer code. The VVP explains the various tests needed to show that the computer code properly performed the functional requirements listed in the RD.

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 DD describes the theoretical model, the mathematical model, and the major components of the software.

The implementation phase consists of developing source code using a programming language (e.g., FORTRAN) or other form suitable for compilation or translation into executable computer software. The design, as described in the DD, 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 ID and the UM. The ID provides the source code listing and describes the process performed to generate executable software, and the UM provides information that assists the user in understanding and using the code.

The verification and 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 UM. One document, the VD, is produced during this phase. The VD documents the test case input and output files and evaluates the results against the acceptance criteria in the VVP.

In the CCA, the DOE used these procedures and documents to show that the PA computer codes calculated numerical models properly, were free of coding errors, and produced stable results. The DOE used the same process and requirements for the CRA-2004 PA computer codes.

23.4.3.6 Peer Review

The DOE performed two peer reviews to support the CRA-2004 PA calculations. These peer reviews evaluated the new spallings model and the minor changes made to the Disposal System Geometry, Repository Fluid Flow, and DRZ conceptual models.

The Spallings Model Peer Review was performed from July 2003 to October 2003; the final report was published in October 2003 (CRA-2004, Appendix PEER-2004, Section PEER-2004-3.1.2). 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. The DOE developed a new numerical code, 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.

The Salado Flow Conceptual Model Peer Review was performed from April 2002 to March 2003; the final report was published in May 2003 (CRA-2004, Appendix PEER-2004, Section PEER-2004-2.1.3). This peer review evaluated changes made to three conceptual models (Disposal System Geometry, Repository Fluid Flow, and DRZ) as a result of (1) new information acquired after the original certification decision; or (2) changes to conceptual model assumptions mandated by the EPA in the final CCA decision, such as the Option D panel closure condition. The changes included: (1) modification of the computational grid to accommodate the new panel closure requirement, (2) shaft simplification, and (3) refinement to the BRAGFLO grid.

23.4.4 EPA's Evaluation of Compliance for the 2004 Recertification

23.4.4.1 Conceptual Models

As in the CCA, all conceptual models used in the CRA-2004 were approved (see Section 23.2.4 for more discussion of the results of the CCA conceptual model peer review) by conceptual model peer reviews that considered whether or not conceptual models represented possible futures of the disposal system. The EPA agreed with the peer review panels and therefore found that the DOE continued to be in compliance with section 194.23(a)(3)(i) (CARD 23, Section "Recertification Decision 194.23(a)(3)," U.S. Environmental Protection Agency 2006f).

23.4.4.2 Mathematical Models

In the evaluation for recertification, the EPA evaluated each of the mathematical models for the computer codes used in the CRA-2004 PA to determine if the governing equations (e.g., flow and transport governing equations), process-related equations (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 PA. CRA-2004, Appendix PA, Section PA-4.0 and UMs and APs for each code were the primary sources of information on the mathematical models employed in PA. In general, mathematical formulations were adequately explained and reasonable. The DOE adequately documented and described simplifications of conceptual models in the CRA-2004 PA. The EPA found that the DOE provided an adequate technical basis to support the mathematical formulations (CARD 23, Section "Recertification Decision 194.23(a)(3)," U.S. Environmental Protection Agency 2006f).

The EPA also reevaluated the functional tests described in the VD for each computer code to ensure that the DOE's tests of the computer codes demonstrated that they performed as specified in the RD. The EPA reviewed the testing of each code to verify that the 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. The EPA found that the DOE continued to comply with 40 CFR § 194.23(a)(3)(ii) (U.S. Environmental Protection Agency 2006c, Section 12.0; 2006j, Section 6.0; 2006i, Section 6.0; CARD 23, Section "Recertification Decision 194.23(a)(3)," U.S. Environmental Protection Agency 2006f).

23.4.4.3 Numerical Models

For the CRA-2004, the EPA reviewed all relevant documentation on numerical models solution schemes, which was primarily contained in the CRA-2004, Appendix PA; APs; and supplementary information (e.g., UMs, VDs). The EPA also reviewed each code's QA documentation package for completeness and technical adequacy.

For the CRA-2004, the EPA reviewed the testing used to qualify each code for use in the CRA-2004 PA. The EPA found that the DOE had adequately set the range of functional tests for each code to verify that the code would perform as expected and provide reasonable results (see each code's VD for details of this testing). The EPA found that the DOE continued to comply with the requirements of 40 CFR § 194.23(a)(3)(iii) (U.S. Environmental Protection Agency 2006c, Section 12.0; 2006j, Section 6.0; 2006i, Section 6.0; CARD 23, Section "Recertification Decision 194.23(a)(3)," U.S. Environmental Protection Agency 2006f).

23.4.4.4 Computer Models

The EPA reviewed all of the relevant documentation (UM, DD, RD, VVP, and VD) pertaining to each of the major codes described above as well as the CRA-2004, Appendix PA and associated attachments. Since the CCA, the EPA also periodically performed an independent review of the DOE's testing of each code to verify that results appeared accurate and free of coding error (U.S. Environmental Protection Agency 2006c, 2006i, and 2006j). The EPA ultimately found that each PA computer code produced results that showed continued compliance with this requirement.

During its review, the EPA questioned whether SANTOS produced results that were an accurate implementation of the numerical models and were free of coding errors (Cotsworth 2004). Specifically, the EPA questioned whether SANTOS was properly tested for accuracy and whether the average stress of less than 5 megapascal that SANTOS predicted for waste was reasonable. In the DOE's response (Detwiler 2004a), the DOE showed that a full functionality test of SANTOS was performed as part of the code qualification and that the results of SANTOS calculations were compared to the results of another computer code called SPECTROM-32. These activities showed that SANTOS produces results adequate for the development of porosity surfaces used in the CRA-2004 PA and was accepted by the EPA (U.S. Environmental Protection Agency 2006l, Section 6.0).

The EPA was able to determine that the CRA-2004 PA computer codes continued to comply with 40 CFR § 194.23(a)(3)(iv) (CARD 23, Section "Recertification Decision 194.23(a)(3)," U.S. Environmental Protection Agency 2006f).

23.4.4.5 Peer Review

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

The EPA examined the peer review plan and the final peer review report for the Spallings Model Peer Review and found that they adequately fulfilled the requirements of section 194.27 and NUREG-1297. The EPA also observed the actual performance of the peer review panel, the selection of the panel members, the interaction of the panel with the DOE, and the documents produced during and as a result of the peer review. The EPA found the process satisfied the requirements of section 194.27 and the guidance in NUREG-1297 (U.S. Environmental Protection Agency 2006d, Section 5.0).

The EPA examined the peer review plan and the final peer review report for the Salado Flow Conceptual Model Peer Review and found that they adequately fulfilled the requirements of section 194.27 and NUREG-1297. The EPA also observed the actual performance of the peer review panel members, the selection of the panel, the interaction of the peer review panel with the DOE, and the documents produced during and as a result of the peer review. The EPA found the process compatible with the requirements of section 194.27 and the guidance in NUREG-1297 (U.S. Environmental Protection Agency 2006e, Section 5.0).

Based on a review and evaluation of the CRA-2004 and supplemental information provided by the DOE, the EPA determined that the DOE continued to comply with the requirements for section 194.23(a)(3)(v) (CARD 23, Section "Recertification Decision 194.23(a)(3)," U.S. Environmental Protection Agency 2006f).

23.4.5 Changes or New Information Since the 2004 Recertification

23.4.5.1 Conceptual Models

All conceptual models used in the CRA-2009 PA were previously peer reviewed. No modifications have been made to the conceptual models since the 2006 recertification decision (see Section 23.3.5 for a discussion of modifications that were proposed, but not included in the CRA-2009). Thus, there is no new information to provide in the CRA-2009 and the DOE continues to demonstrate compliance with the provision of section 194.23(a)(3)(i).

23.4.5.2 Mathematical Models

No changes were made in the methodology used to document mathematical models and initial and boundary conditions from the CRA-2004. Discussion of the mathematical models and initial and boundary conditions are found in Appendices PA-2009, PORSURF-2009, SOTERM-2009, and TFIELD-2009. UMs and APs are also used to document mathematical models and the initial and boundary conditions for the CRA-2009. Table 23-4 lists the APs for the CRA-2009 PA.

Table 23-4. APs for the CRA-2009 PA

AP	Reference
Parameters	Kirchner 2008a; Fox 2008
Cuttings & Cavings	Ismail 2008
Spallings	Vugrin 2005; Ismail 2008
Direct Brine Release	Clayton 2008
Actinide Mobilization	Garner and Leigh 2005
Salado Flow	Nemer and Clayton 2008
Salado Transport	Ismail and Garner 2008
Culebra Flow	Lowry and Kanney 2005
Culebra Transport	Lowry and Kanney 2005
Normalized Release	Dunagan 2008
Sensitivity Study	Kirchner 2008b
Summary	Clayton et al. 2008

No new codes have been added to the WIPP PA since the CRA-2004 PABC. Two codes, BRAGFLO and NUTS, were modified for the CRA-2009 PA. BRAGFLO was modified from version 5.0 to version 6.0 to incorporate additional capabilities and flexibility (Nemer 2006). The UM (Nemer 2007a), RD/VVP (Nemer 2007b), ID (Nemer 2007c), and VD (Nemer 2007d) were generated for BRAGFLO version 6.0. NUTS version 2.05a had a time and date incompatibility with the upgraded operating system (Gilkey 2006), so it was modified to version 2.05c. The only difference between version 2.05a and 2.05c is the change made to correct the time and date incompatibility. As this was a minor code change, only the ID (Gilkey 2006) was updated and no changes were made to the UM, RD/VVP, or VD.

The DOE continues to provide documentation that mathematical models incorporate equations and boundary conditions that reasonably represent the mathematical formulation of the conceptual models, and thus continues to demonstrate compliance with the provision of section 194.23(a)(3)(ii).

23.4.5.3 Numerical Models

As in the CRA-2004, the information used to evaluate the stability of the numerical schemes was provided in the VDs and APs that the DOE prepared for each of the CRA-2009 PA computer codes. Therefore, the DOE continues to provide documentation that numerical models provide numerical schemes that enable the mathematical models to obtain stable solutions and thus continues to demonstrate compliance with the provisions of section 194.23(a)(3)(iii).

23.4.5.4 Computer Models

As in the CRA-2004, the information used to show that the PA computer codes calculated numerical models properly and that the computer codes were free of coding errors and produced stable results was provided in the RD/VVP and VD prepared for each of the CRA-2009 PA computer codes. Therefore, the DOE continues to provide documentation that computer models accurately implement the numerical models and thus, continues to demonstrate compliance with the provision of section 194.23(a)(3)(iv).

23.4.5.5 Peer Review

No additional peer review results since the 2006 recertification decision have been included in the CRA-2009 PA calculations (see Section 23.3.5 for a discussion of modifications that were proposed, but not included, in the CRA-2009). Thus, there is no new information to provide in the CRA-2009, and the DOE continues to demonstrate compliance with the provision of section 194.23(a)(3)(v).

23.5 40 CFR § 194.23(b)

23.5.1 Background

40 CFR § 194.23(b) requires that computer codes be documented in accordance with an appropriate quality assurance standard.

23.5.2 1998 Certification Decision

In the CCA, to meet the requirements of section 194.23(b), the DOE provided documentation of compliance with quality assurance requirements of American Society of Mechanical Engineers (ASME) Nuclear Quality Assurance (NQA)-2a-1990 addenda, Part 2.7, to ASME NQA-2-1989 edition. This documentation included plans for QA software, software requirements documentation, software design and implementation documentation, software verification and validation documentation, and user documentation. Based on the EPA audits and the CCA review, the EPA found the DOE in compliance with the requirements of section 194.23(b).

A complete description of the EPA's 1998 Certification Decision for section 194.23(b) can be obtained from CARD 23, Section 8.4 (U.S. Environmental Protection Agency 1998a).

23.5.3 Changes in the CRA-2004

The CRA-2004, Chapter 5.0 describes the DOE's QA program. Software QA is described in the CRA-2004, Chapter 5.0, Section 5.3.20. The DOE's QA program, dated May 2003, is contained in the CRA-2004, Appendix QAPD. Section 6 of the DOE QAPD incorporated the requirements of ASME NQA-2a-1990 addenda, Part 2.7, to ASME NQA-2-1989 edition. See CARD 22, U.S. Environmental Protection Agency (2006k), for further discussion of the EPA's review of the DOE's approach to the QA requirements for computer codes and models.

23.5.4 EPA's Evaluation of Compliance for the 2004 Recertification

The EPA verified compliance with the requirements of 40 CFR § 194.22(a)(2)(iv) by reviewing Section 6.0 of the Carlsbad Field Office QAPD and conducting periodic inspections of the Sandia National Laboratories (SNL) and Washington TRU Solutions QA programs since the CCA decision. The DOE's documentation included plan(s) for software QA, software requirements documentation, software design and implementation documentation, software verification and validation documentation, and user documentation. The EPA found that the DOE's QA requirements for computer codes used in the PA and compliance assessment continued to be in agreement with those specified in 40 CFR § 194.22, and that their code documentation was adequate. See CARD 22, Section "Evaluation of Compliance for Recertification" (U.S. Environmental Protection Agency 2006k), for further discussion of the EPA's review.

Based on a review and evaluation of the CRA-2004 and supplemental information provided by the DOE, the EPA determined that the DOE continued to comply with the requirements for section 194.23(b) (CARD 23, Section "Recertification Decision 194.23(b)," U.S. Environmental Protection Agency 2006f).

23.5.5 Changes or New Information Since the 2004 Recertification

The documentation standards of the computer codes have not changed since the CRA-2004 decision. Thus, there is no new information to provide in the CRA-2009, and the DOE continues to demonstrate compliance with the provision of section 194.23(b).

23.6 40 CFR § 194.23(c)(1)

23.6.1 Background

40 CFR § 194.23(c)(1) requires documentation of all models and computer codes, including descriptions of the theoretical backgrounds and the method of analysis for each model.

23.6.2 1998 Certification Decision

In the CCA, the DOE provided documentation of all models and computer codes, including descriptions of the theoretical backgrounds and the method of analysis for each model. The EPA's evaluation found that the CCA and supplementary information provided an adequate description of the theoretical backgrounds and method of analysis for each model used in the calculations. The DOE's documentation of conceptual models, alternative conceptual models, and the Conceptual Models Peer Review Panel is discussed in CARD 23 Sections 1.4, 2.4, and 7.4, respectively (U.S. Environmental Protection Agency 1998a).

A complete description of the EPA's 1998 Certification Decision for section 194.23(c)(1) can be obtained from CARD 23, Section 9.4 (U.S. Environmental Protection Agency 1998a).

23.6.3 Changes in the CRA-2004

Most of the major codes used for modeling the PA in the CRA-2004 had not changed since the CCA. Codes added to the CRA-2004 PA since the CCA were MODFLOW, PEST, and DRSPALL. Each of the CRA-2004 PA codes is documented in its own UM, AP, RD, VVP, DD, ID, and VD (see Section 23.4.3.1 for a summary of each document). The DOE used these documents as the primary vehicles to describe the conceptual models, mathematical models, and numerical methods that provided the basis for the theory and the assumptions underlying the computer codes. The DOE included additional documentation in various appendices to the CRA-2004 (e.g., CRA-2004, Appendix PA, Attachment MASS and Attachment SOTERM). The DOE's documentation also contained justification for the use of the models, conceptual model derivation, mathematical derivations, and solution methods used in the codes (see the CRA-2004, Chapter 6.0 and Appendix PA).

23.6.4 EPA's Evaluation of Compliance for the 2004 Recertification

The primary codes that the EPA reviewed include: CUTTINGS_S, MODFLOW, SECOTP2D, SUMMARIZE, PRECCDFGF, CCDFGF, LHS, DRSPALL, PANEL, BRAGFLO, NUTS, FMT, PEST, SANTOS, and ALGEBRA. The EPA found the DOE's description of the theoretical background of each code, provided primarily in the UM and AP, to be adequate. With respect to the documentation pertaining to the method of analysis, the EPA found the descriptions in the AP for each code to be sufficiently complete.

For the CRA-2004, the EPA reevaluated all available documentation on each of the computer codes for completeness, clarity, and logical development of the theoretical bases for 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 (1) formulated on a sound theoretical foundation, and (2) used properly in the PA analysis.

The EPA reviewed all of the relevant documentation pertaining to the theoretical development and application of the models. For further discussion of the EPA's review of documentation for conceptual models, alternative conceptual models, and the Conceptual Models Peer Review Panel, see Section 23.2, Section 23.3, and Section 23.4. The majority of the information was located in the UM and AP for each code. For the CRA-2004, the DOE's theoretical background for almost all of the codes had not changed since the CCA decision. Since the CCA, the DOE had continued to test the PA codes to verify that they still perform as they did during the CCA. The EPA had periodically reviewed and inspected these activities to verify that the PA codes continue to produce adequate results (U.S. Environmental Protection Agency 2006i and 2006j). The CRA-2004, Appendix PA included the theoretical background, mathematical development, and numerical development of the main PA codes and its use in the CRA-2004 PA analyses.

After the execution of the original CRA-2004 PA, the 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. The EPA requested that the DOE verify that these errors had been corrected and that the codes passed the correct information to assure the analysis methods and assessments achieve correct results (Cotsworth 2005). The DOE modified the codes, corrected the analysis process, and retested to confirm that the errors had been corrected. The DOE also reran parts of the original CRA-2004 PA to assess the impact of these corrections. The EPA found that the DOE had corrected the errors and verified that the code obtained the correct data to perform their analysis for the CRA-2004 PABC (U.S. Environmental Protection Agency 2006c, Section 12.0). The EPA found that the DOE's level of documentation continued to be consistent with the adequate level of documentation produced during the CCA review, and that the DOE continued to be in compliance with section 194.23(c)(1) (CARD 23, Section "Recertification Decision 194.23(c)," U.S. Environmental Protection Agency 2006f).

23.6.5 Changes or New Information Since the 2004 Recertification

No changes were made to the documentation procedure of PA computer codes used in the CRA-2009. Thus, there is no new information to be provided as part of the CRA-2009, and the DOE continues to demonstrate compliance with the provisions of section 194.23(c)(1).

23.7 40 CFR § 194.23(c)(2)

23.7.1 Background

40 CFR § 194.23(c)(2) requires (1) general descriptions of the models; (2) discussions on the limits of applicability of each model; (3) detailed instructions for executing the computer codes, including hardware and software requirements; (4) input and output formats with explanations of each input and output variable and parameter (e.g., parameter name and units); (5) listings of input and output files from a sample computer run; and (6) reports on code verification, benchmarking, validation, and QAPs.

23.7.2 1998 Certification Decision

In the CCA, the DOE provided 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. The EPA's evaluation found that the CCA and supplementary information included (1) an adequate description of each model used in the calculations; (2) a description of limits of applicability of each model; (3) detailed instructions for executing the computer codes; (4) hardware and software requirements to run these codes; (5) input and output formats with explanations of each input and output variable and parameter; (6) listings of input and output files from sample computer runs; and (7) reports of code verification, benchmarking, validation, and QAPs.

A complete description of the EPA's 1998 Certification Decision for section 194.23(c)(2) can be obtained from CARD 23, Section 10.4 (U.S. Environmental Protection Agency 1998a).

23.7.3 Changes in the CRA-2004

As in the CCA, documentation for the CRA-2004 regarding the DOE's compliance with section 194.23(c)(2) is primarily contained in the UM, AP, VD, ID, DD, RD, and VVP for each code. Table 23-5 lists the requirements of section 194.23(c)(2) and where these requirements are addressed in the DOE documents.

23.7.4 EPA's Evaluation of Compliance for the 2004 Recertification

The EPA reviewed all of the relevant documentation pertaining to requirements specified in section 194.23(c)(2) for the following codes: CUTTINGS_S, MODFLOW, SECOTP2D, CCDFGF, LHS, PANEL, BRAGFLO, NUTS, FMT, PEST, DRSPALL, SANTOS, and ALGEBRA (U.S. Environmental Protection Agency 2006c; 2006i; and 2006j). The DOE's code documentation provided enough information for the EPA to understand and execute the models, determine the possible impact of any assumptions, and verify that the codes were tested and quality assured.

The DOE replaced the SECOFL2D flow code used in the CCA with the MODFLOW-2000 flow code. The primary reasons given for the change are (1) that MODFLOW-2000 is well supported by a large user base and is continuing to be developed, while SECOFL2D is not; (2) MODFLOW is designed to operate on multiple computer platforms, while SECOFL2D was designed to work on only the VAX/Alpha platforms; and (3) the new pilot point estimation code, PEST, was designed to use only MODFLOW-2000 (Detwiler 2004b). The EPA determined that MODFLOW-2000 is a reasonable replacement to SECOFL2D and that the MODFLOW/PEST T field estimate combination is a significant improvement over the SECOFL2D/GRASP-INV combination used in the CCA (U.S. Environmental Protection Agency 2006c). The EPA determined that the DOE continued to demonstrate compliance with section 194.23(c)(2) (CARD 23, Section "Evaluation of Compliance for Recertification 194.23(c)," U.S. Environmental Protection Agency 2006f).

Table 23-5. Location of Documentation for Models and Computer Codes Used in PA

Requirement in Compliance Application Guidance	Document Containing Information						
	UM	AP	VD	ID	DD	RD/VVP	SNL QA Procedures[a]
General descriptions of the models	X	X	—	—	X	—	—
Discussions of the limits of applicability of each model	X	X	—	—	X	—	X
Detailed instructions for executing the computer codes	—	X	—	X	X	—	X
Hardware requirements for executing the computer codes	X	X	—	X	—	—	X
Software requirements for executing the computer codes	X	X	—	—	—	—	X
Input and output formats with explanations of each input and output variable and parameter	X	X	—	—	X	—	—
Listings of input and output files from a sample computer run	X	X	—	—	—	—	X
Reports on code verification	—	X	X	—	—	X	X
Reports on benchmarking	—	X	X	—	—	X	X
Reports on validation	—	X	X	—	—	X	X
Reports on QAPs	—	X	—	—	—	—	X

X = Information meeting the requirement is found in this document.

[a] See the CRA-2004, Appendix QAPD, Section 6.0.

23.7.5 Changes or New Information Since the 2004 Recertification

No changes were made to the documentation procedure of PA computer codes used in the CRA-2009. Thus, there is no new information to provide in the CRA-2009, and the DOE continues to demonstrate compliance with provision of section 194.23(c)(2).

23.8 40 CFR § 194.23(c)(3)

23.8.1 Background

40 CFR § 194.23(c)(3) requires detailed descriptions of the computer code structures and a complete listing of computer source codes.

23.8.2 1998 Certification Decision

In the CCA, the DOE provided detailed descriptions of the computer code structure and a complete listing of computer source codes. The EPA's evaluation found that the CCA and supplementary information adequately provided a detailed description of the computer code structures and supplied a complete listing of the computer source code in supplementary documentation to the CCA. The documentation of computer codes described the structure of computer codes with sufficient detail to allow the EPA to understand how software subroutines are interrelated. The code structure documentation shows how the codes operate to provide accurate solutions of the conceptual models.

A complete description of the EPA's 1998 Certification Decision for section 194.23(c)(3) can be obtained from CARD 23, Section 11.4 (U.S. Environmental Protection Agency 1998a).

23.8.3 Changes in the CRA-2004

The ID for each modeling code contains the information relevant to compliance with section 194.23(c)(3). The ID provides the information necessary for the recreation of the code as used in the CRA-2004 PA calculation. With this information, the user can compile the source code and install it on a computer system identical to that used in the CRA-2004 calculations. The ID also includes the source code listing and code compilation information.

23.8.4 EPA's Evaluation of Compliance for the 2004 Recertification

The EPA reviewed all of the relevant documentation, and 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, NUTS, FMT, PEST, SANTOS, DRSPALL, SUMMARIZE, and ALGEBRA. The EPA found that the DOE submitted all of the source code listings. The 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 the EPA to understand how software subroutines were linked and how to execute the PA. The EPA determined that the DOE continues to demonstrate compliance with section 194.23(c)(3) (CARD 23, Section "Recertification Decision 194.23(c)," U.S. Environmental Protection Agency 2006f).

23.8.5 Changes or New Information Since the 2004 Recertification

No changes were made to the documentation procedure of PA computer codes used in the CRA-2009. The DOE continues to demonstrate compliance with the provisions of section 194.23(c)(3).

23.9 40 CFR § 194.23(c)(4)

23.9.1 Background

40 CFR § 194.23(c)(4) requires detailed descriptions of data collection, data reduction and analysis, and code input parameters development.

23.9.2 1998 Certification Decision

In the CCA, the DOE provided detailed descriptions of data collection, data reduction and analysis, and code input parameters development. The EPA's evaluation found that the CCA and supplementary information adequately (1) provided a detailed listing of the code input parameters; (2) listed sampled input parameters; (3) provided a description of parameters and the codes in which they are used; (4) discussed parameters important to releases; (5) described data collection procedures, sources of data, data reduction and analysis; and (6) described code input parameter development, including an explanation of QA activities.

A complete description of the EPA's 1998 Certification Decision for section 194.23(c)(4) can be obtained from the CARD 23, Section 12.4 (U.S. Environmental Protection Agency 1998a).

23.9.3 Changes in the CRA-2004

The primary sources of CRA-2004 parameter information are in the CRA-2004, Chapter 6.0 (especially Tables 6-10 to 6-30), Appendix PA, Attachment PAR, and other appendices describing specific computer codes and parameter records. Records of parameters for the CRA-2004 included the following:

- SNL Form NP 9-2-1 WIPP Parameter Entry Form (PEF): All PA parameters are defined using this form, which contains the numerical values and distributions of parameters used as input to PA codes, identifies the code the parameter is used in, and includes information to trace the development of each parameter. The PEF replaced Form 464 used in the CCA PA.

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

- Data Records Packages (DRP): These documents are typically generated for parameters 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 repository). These packages are generally the first step that links the development of a parameter from the measured data to the values used in the PA.

- APs: These are supplementary documents that generally describe all parameters used by a particular code in the PA calculations.

The main source for parameter documentation is the PEF. The need for further documentation in the other three types of documents depends upon the nature of the parameter, such as whether it is a widely accepted chemical constant (e.g., atomic weight of an isotope) or a value requiring experimental data for verification. Table 23-6 describes the types of information found in each of these four documents and possible paths in documenting parameter record information.

The CCA contained approximately 1,600 parameters and the CRA-2004 contained approximately 1,700 parameters consisting of numerical values or ranges of numerical values that describe different physical and chemical aspects of the repository, the geology and geometry of the area surrounding the WIPP, and possible scenarios for human intrusion. Some parameters are well-established chemical constants, such as Avogadro's number or the universal gas constant. Other parameters describe attributes unique to the WIPP, such as the solubility and mobility of specific actinides in brines in the WIPP. An example of a parameter related to the geology of the WIPP is the permeability of the rock in the Culebra above the WIPP. The 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.

In the documents described above, the DOE described the methods that develop and support the approximately 1,700 parameters used in the CRA-2004. All of the documents listed above are used to explain the full development of parameter values used as inputs to the PA calculations. Table 23-6 indicates the documents that contain information required under section 194.23(c)(4).

23.9.4 EPA's Evaluation of Compliance for the 2004 Recertification

The EPA, as for the CCA, performed a thorough review of the parameters and parameter development process for the CRA-2004. For the CRA-2004 parameter review, the EPA focused its review on parameters that had changed or were new since the CCA. The EPA's review of the parameters and parameter development is described in detail (U.S. Environmental Protection Agency 2006m, 2006n). The EPA reviewed parameter packages for a sample of approximately 1,700 parameters used in the CRA-2004 PA calculations. The parameter records include WIPP PEFs (NP 9-2-1), requestor documents or forms, DRPs, and APs.

The EPA's review of PA parameters took place in three phases. In 2003, the EPA reviewed the transfer of parameters from the CCA database to a new database system (U.S. Environmental Protection Agency 2006n). Next, the EPA reviewed the parameters changed as a result of the parameter transfer to the CRA-2004 PA calculations (U.S. Environmental Protection Agency 2006n). The 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 spallings code, DRSPALL. The EPA was able to verify that the new and changed parameters were adequately recorded in the WIPP parameter database and that most of these parameters were justified and traceable to adequate supporting documentation. Finally, the EPA reviewed the parameter changes and documentation for values changed for the CRA-2004 PABC calculations required by the EPA to confirm the impact of code errors and parameter changes on the PA compliance results (U.S. Environmental Protection Agency 2006m).

The EPA found minor concerns at each phase of the review. Ultimately, the DOE corrected each concern, and the EPA verified that parameters used in the CRA-2004 were adequately developed, documented, and traceable. The EPA determined that the DOE continued to comply with section 194.23(c)(4) (CARD 23, Section "Recertification Decision 194.23(c)," U.S. Environmental Protection Agency 2006f).

During the EPA's completeness review, stakeholders commented on the drilling rate used in the CRA-2004 PA calculations. During meetings with stakeholders in July of 2004, comments arose regarding the drilling rate used in the CRA-2004 and suggested that a number twice the existing rate should be used in PA calculations. In a December 3, 2004 email, the EPA informed the DOE that they were required to evaluate the impact of using twice the CRA-2004 PA drilling

Table 23-6. Location of Required Information on Parameters Used in Codes for PA

Requirement in Compliance Application Guidance	Document Containing Information							
	PEF	PIRP	DRP	AP	CRA-2004[a]	Att. PAR[b]	App. QAPD[c]	Parameter Database
Detailed listings of code input parameters	—	—	—	—	—	—	—	X
Detailed listings of the sampled parameters	—	—	—	—	—	X	—	X
Codes in which the parameters were used	X	—	—	X	—	—	—	X
Computer code names of the sampled parameters	X	—	—	X	—	—	—	X
Descriptions of the data sources	X	X	X	X	—	—	—	X
Descriptions of the parameters	—	—	—	X	X	X	—	X
Descriptions of the data collection procedures	—	X	X	—	—	—	—	—
Description of the data reduction and analysis	—	X	X	X	—	—	—	—
Descriptions of code input parameter development	—	—	X	—	—	—	—	—
Discussions of the linkage between input parameter information and data used to develop the input information	—	X	X	X	—	—	—	X
Discussions of the importance of the sampled parameters relative to final releases	—	—	—	X	—	—	—	—
Discussions of correlations among sampled parameters and how these are addressed in PA	—	—	—	—	—	X	—	—
Listing of the data sources used to establish parameters (e.g., experimentally derived, standard textbook values)	X	X	X	X	—	—	—	X
Data reduction methodologies used for PA parameters	—	X	X	X	—	—	—	—
Explanation of QA activities	—	—	—	—	X	—	X	—

X = Information meeting the requirement is found in this document.

[a] See CRA-2004, Chapter 6.0 for parameter descriptions and CRA-2004, Chapter 5.0 for an explanation of QA activities.

[b] CRA-2004, Appendix PA, Attachment PAR.

[c] CRA-2004, Appendix QAPD.

rate. The analysis was conducted and the DOE documented the results (Kanney and Kirchner 2004). The EPA reviewed the DOE's response and noted that doubling the drilling rate does increase predicted releases, but that the results are still well within regulatory release limits.

Ultimately, the EPA was able to determine that the DOE continued to be in compliance with section 194.23(c)(4) (CARD 23, Section "Recertification Decision 194.23(c)," U.S. Environmental Protection Agency 2006f).

23.9.5 Changes or New Information Since the 2004 Recertification

For the CRA-2009, there are 90 new parameters and 15 modified parameters (Fox 2008, Table 6). The 15 modified parameters and 10 of the 90 new parameters are a result of corrections and parameter updates. The remaining 80 new parameters arose from the capability improvements added to the BRAGFLO computer code. More discussion of the CRA-2009 parameters is found in Fox (2008).

As in the CRA-2004, the information used to show detailed descriptions of data collection procedures, data reduction and analysis, and code input parameter development was provided in the PEFs that the DOE prepared for each of the CRA-2009 PA parameters (see Fox 2008). Therefore, the DOE continues to provide documentation of the parameter development and thus continues to demonstrate compliance with the provision of section 194.23(c)(4).

23.10 40 CFR § 194.23(c)(5)

23.10.1 Background

40 CFR § 194.23(c)(5) requires documentation of any necessary licenses for all models and computer codes.

23.10.2 1998 Certification Decision

The DOE did not use any software that requires a license, so the EPA found that the DOE demonstrated compliance with section 194.23(c)(5).

A complete description of the EPA's 1998 Certification Decision for section 194.23(c)(5) can be obtained from CARD 23, Section 13.1 (U.S. Environmental Protection Agency 1998a).

23.10.3 Changes in the CRA-2004

As in the CCA, no licenses from software vendors were required to operate the codes essential for the WIPP PA. Most of the computer codes for the WIPP PA were developed and programmed by the DOE 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.

23.10.4 EPA's Evaluation of Compliance for the 2004 Recertification

As the DOE did not use any software that requires a license, the EPA determined that the DOE continued to comply with section 194.23(c)(5) (CARD 23, Section "Recertification Decision 194.23(c)," U.S. Environmental Protection Agency 2006f).

23.10.5 Changes or New Information Since the 2004 Recertification

No new codes were added for the CRA-2009 PA and no software requiring a license was used. Thus, there is no new information to provide in the CRA-2009, and the DOE continues to demonstrate compliance with the provisions of section 194.23(c)(5).

23.11 40 CFR § 194.23(c)(6)

23.11.1 Background

40 CFR § 194.23(c)(6) requires an explanation of the manner in which models and computer codes incorporate the effects of parameter correlation.

23.11.2 1998 Certification Decision

In the CCA, the DOE provided an explanation of the manner in which models and computer codes incorporate the effects of parameter correlation. The EPA's evaluation found that the CCA and supplementary information adequately discussed how the effects of parameter correlation are incorporated, explained the mathematical functions that describe these relationships, and described the potential impacts on the sampling of uncertain parameters. The CCA also adequately documented the effects of parameter correlation for both conceptual models and the formulation of computer codes, and appropriately incorporated these correlations in the PA.

A complete description of the EPA's 1998 Certification Decision for section 194.23(c)(6) can be obtained from CARD 23, Section 14.4 (U.S. Environmental Protection Agency 1998a).

23.11.3 Changes in the CRA-2004

User-specified parameter correlations for sampled parameters were introduced into the CRA-2004 PA calculations using the Latin Hypercube Sampling (LHS) computer program. The DOE used two types of parameter correlations: user-specified and induced. User-specified (explicit) parameter correlations are input to the LHS computer code using a correlation matrix (or table).

When values 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 parameter correlation in the WIPP PA.

The DOE implemented parameter correlations in the WIPP PA using the LHS computer code (CRA-2004, Appendix PA, Section PA-5.4). CRA-2004 parameter correlations are described in the CRA-2004, Appendix PA, Attachment PAR, Section 4.0.

23.11.4 EPA's Evaluation of Compliance for the 2004 Recertification

The EPA determined that parameter correlations were adequately explained in the CRA-2004, Appendix PA, Attachment PAR, Section PAR-4.0 and were adequately incorporated. The 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. The EPA determined that the DOE continued to comply with section 194.23(c)(6) (CARD 23, Section "Recertification Decision 194.23(c)," U.S. Environmental Protection Agency 2006f).

23.11.5 Changes or New Information Since the 2004 Recertification

The description of the parameter correlations used in the CRA-2009 PA can be found in Fox (2008, Section 4.0). No changes were made in the parameter correlations since the CRA-2004 PABC, except that the conditional relationship between the inundated and humid microbial cellulose degradation rates was modified from the CRA-2004 PABC methodology. For the CRA-2004 PABC, the conditional relationship was enforced in the preprocessing step for the BRAGFLO calculations by setting the humid rate equal to the inundated rate if the sampled humid rate was higher than the inundated rate for a single vector. Changing these values this way introduced a small error into the sensitivity analysis because the regression analysis was based on the sampled value rather than the conditional values.

For the CRA-2009 PA, a conditional relationship was applied so that the sampled inundated rate is used as the maximum in the sampling for the humid rate. This conditional relationship results in a correlation of 0.74 between the humid and inundated rates (Kirchner 2008a). The conditional relationship was applied during the LHS process. The LHSEDIT utility was developed to account for this conditional relationship. The implementation and verification of the LHSEDIT utility is discussed in Kirchner (2008a).

The DOE continues to provide an explanation of the manner in which models and computer codes incorporate the effects of parameter correlation and thus demonstrate compliance with the provisions of section 194.23(c)(6).

23.12 40 CFR § 194.23(d)

23.12.1 Background

The DOE must provide the EPA free access to PA models and computer codes.

23.12.2 1998 Certification Decision

During the review of the CCA, the DOE provided the EPA with ready access to computer hardware required to perform independent computer simulations. Therefore, the EPA found the DOE in compliance with the requirements of 40 CFR § 194.23(d).

A complete description of the EPA's 1998 Certification Decision for section 194.23(d) can be obtained from CARD 23, Section 15.4 (U.S. Environmental Protection Agency 1998a).

23.12.3 Changes in the CRA-2004

No specific changes were made to the CRA-2004 to demonstrate compliance with section 194.23(d). The DOE provided access for the EPA during the CRA-2004 to PA models and computer codes.

23.12.4 EPA's Evaluation of Compliance for the 2004 Recertification

The EPA expected the DOE to identify points of contact to facilitate the process for the EPA to perform independent simulations, provide ready access to the hardware and software needed to perform simulations related to the CRA-2004 evaluation, and assist the EPA personnel in exercising the DOE computer codes.

The DOE provided contacts to assist the EPA in operating the hardware needed to perform the independent computer simulations necessary to verify the simulations related to the CRA-2004. The DOE provided the EPA and authorized personnel with unrestricted access to this computer hardware and software.

Based on adequate support and access to PA computer codes, input files, and PA-related documentation, the EPA determined that the DOE continued to comply with the requirements for section 194.23(d) (CARD 23, Section "Recertification Decision 194.23(d)," U.S. Environmental Protection Agency 2006f).

23.12.5 Changes or New Information Since the 2004 Recertification

No specific changes were made to the CRA-2009 to demonstrate compliance with section 194.23(d). Thus, the DOE will continue to provide the EPA with unrestricted access to the computer hardware and software and the DOE continues to demonstrate compliance with the provisions of section 194.23(d).

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