40 CFR Part 191
Subparts B and C
Compliance Recertification Application-2026
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

Compliance Recertification Application 2026
Models and Computer Codes
(40 CFR 194.23)

TABLE OF CONTENTS

23.0 MODELS AND COMPUTER CODES (40 CFR 194.23) 23-1
23.1 Requirements 23-1
23.2 Background 23-2
23.3 40 CFR 194.23(a)(1) 23-2
23.3.1 Background 23-2
23.3.2 Description of Conceptual Models 23-2
23.3.2.1 Description of Scenarios 23-5
23.3.3 Changes or New Information for the CRA-2019 DPA 23-5
23.3.4 Changes or New Information Since the CRA-2019 DPA 23-5
23.4 40 CFR 194.23(a)(2) 23-5
23.4.1 Background 23-5
23.4.2 Changes or New Information for the CRA-2019 DPA 23-6
23.4.3 Changes or New Information Since the CRA-2019 DPA 23-6
23.5 40 CFR 194.23(a)(3) 23-6
23.5.1 Background 23-6
23.5.2 Documentation 23-7
23.5.3 Changes or New Information for the CRA-2019 DPA 23-8
23.5.3.1 Conceptual Models 23-8
23.5.3.2 Mathematical Models 23-8
23.5.3.3 Numerical Models 23-9
23.5.3.4 Computer Codes 23-9
23.5.3.5 Peer Review 23-9
23.5.4 Changes or New Information Since the CRA-2019 DPA 23-9
23.5.4.1 Conceptual Models 23-9
23.5.4.2 Mathematical Models 23-9
23.5.4.3 Numerical Models 23-10
23.5.4.4 Computer Codes 23-10
23.5.4.5 Peer Review 23-10
23.6 40 CFR 194.23(b) 23-11
23.6.1 Background 23-11
23.6.2 Changes or New Information for the CRA-2019 DPA 23-11
23.6.3 Changes or New Information Since the CRA-2019 DPA 23-11
23.7 40 CFR 194.23(c)(1) 23-11
23.7.1 Background 23-11
23.7.2 Changes or New Information for the CRA-2019 DPA 23-11
23.7.3 Changes or New Information Since the CRA-2019 DPA 23-12
23.8 40 CFR 194.23(c)(2) 23-12
23.8.1 Background 23-12
23.8.2 Changes or New Information for the CRA-2019 DPA 23-12
23.8.3 Changes or New Information Since the CRA-2019 DPA 23-12
23.9 40 CFR 194.23(c)(3) 23-12
23.9.1 Background 23-12

23.9.2 Changes or New Information for the CRA-2019 DPA 23-12
23.9.3 Changes or New Information Since the CRA-2019 DPA 23-13
23.10 40 CFR 194.23(c)(4) 23-13
23.10.1 Background 23-13
23.10.2 Changes or New Information for the CRA-2019 DPA 23-13
23.10.3 Changes or New Information Since the CRA-2019 DPA 23-13
23.11 40 CFR 194.23(c)(5) 23-13
23.11.1 Background 23-13
23.11.2 Changes or New Information for the CRA-2019 DPA 23-14
23.11.3 Changes or New Information Since the CRA-2019 DPA 23-14
23.12 40 CFR 194.23(c)(6) 23-14
23.12.1 Background 23-14
23.12.2 Changes or New Information for the CRA-2019 DPA 23-14
23.12.3 Changes or New Information Since the CRA-2019 DPA 23-14
23.13 40 CFR 194.23(d) 23-14
23.13.1 Background 23-14
23.13.2 Changes or New Information for the CRA-2019 DPA 23-15
23.13.3 Changes or New Information Since the CRA-2019 DPA 23-15
23.14 References 23-15

LIST OF TABLES

Table 23-1. WIPP Conceptual Models 23-3

ACRONYMS AND ABBREVIATIONS

AP	Analysis Package
APPA	Additional Panels Performance Assessment
ASME	American Society of Mechanical Engineers
CCA	Compliance Certification Application
CFR	Code of Federal Regulations
CRA	Compliance Recertification Application
DD	Design Document
DOE	U.S. Department of Energy
DPA	Deferred Performance Assessment
DRZ	Disturbed Rock Zone
EPA	U.S. Environmental Protection Agency
FEPs	Features, Events, and Processes
ID	Implementation Document
NQA	Nuclear Quality Assurance
PA	Performance Assessment
RD	Requirements Document
RPPCR	Replacement Panels Planned Change Request
SNL	Sandia National Laboratories
UM	User's Manual
VD	Validation Document
VVP	Verification and Validation Plan
WIPP	Waste Isolation Pilot Plant

23.0 MODELS AND COMPUTER CODES (40 CFR 194.23)

Title 40 Code of Federal Regulations (CFR) 194.23 (U.S. EPA 1996) presents the requirements for all models and computer codes used in the performance assessment (PA) that the U.S. Department of Energy (DOE) must use to demonstrate compliance with the containment requirements at 40 CFR 191.13 (U.S. EPA 1993). As directed in 40 CFR 194.15(b), where information remains valid and has been submitted in previous recertification applications, such information may be summarized and referenced.

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 Background

The 2026 Compliance Recertification Application (CRA-2026) is based on the interim (12-panel) approved state of the repository. A supplemental PA for the expected final state of the repository (19-panel) has also been executed for the CRA-2026. The information in this section applies to both the approved interim state and final state of the repository. The PAs for the CRA-2026 are developed from the PA used for the Replacement Panels Planned Change Request (RPPCR), which is based on the PA used for the CRA-2019. The PA for the CRA-2019 was deferred and submitted to the U.S. Environmental Protection Agency (EPA) after submittal of the CRA-2019 (U.S. DOE 2019). Consequently, Section 23.0 of the CRA-2019 does not fully describe changes made to the PA since the CRA-2014. In this section, we summarize, separately, changes to the PA up to the CRA-2019 deferred performance assessment (DPA) and changes made since the CRA-2019 DPA.

23.3 40 CFR 194.23(a)(1)

23.3.1 Background

The criteria in 40 CFR § 194.23(a)(1) (U.S. EPA 1996) require descriptions of the conceptual models and scenario construction used to demonstrate compliance. A conceptual model is a set of qualitative assumptions used to describe a system or subsystem for a specific purpose (U.S. DOE 1996, Appendix PEER, Section 2.4). A scenario is a set of possible future conditions of the repository system (U.S. DOE 1996, Section 6.1.4) that are primarily defined by the future occurrence of events.

Conceptual models and scenarios are developed from and refined through the analysis of features, events and processes (FEPs). For this reason, FEP changes and screening analyses are summarized with changes to conceptual models and scenarios.

23.3.2 Description of Conceptual Models

There have been 24 conceptual models developed to describe the Waste Isolation Pilot Plant (WIPP) disposal system (see Table 23-1). There were no name changes to the 24 conceptual models for CRA-2019 (U.S. DOE 2019), and none since. However, three conceptual model implementations have been modified and peer reviewed since the CRA-2019.

Table 23-1. WIPP Conceptual Models

	Conceptual Model	Summary ‡
1	Disposal System Geometry*	Defines the three-dimensional layout of waste panels, drifts, shafts, interbeds, and surrounding formations in a simplified computational grid for flow and transport modeling.
2	Culebra Hydrogeology	Represents the Culebra as a horizontally confined, heterogeneous, double-porosity aquifer, with transmissivity fields calibrated to observed heads and used for steady-state flow.
3	Repository Fluid Flow*	Models multiphase brine and gas movement within the excavated rooms and surrounding rock (DRZ, interbeds, shafts) using Darcy's law and two-phase flow theory.
4	Salado	Treats the Salado formation as layered halite and anhydrite porous media that provide the principal natural barrier to fluid exchange with the repository.
5	Impure Halite	Represents intact halite-rich Salado rock with uniform, constant bulk properties (porosity, permeability).
6	Salado Interbeds	Explicitly models three anhydrite interbeds with pressure-dependent fracture dilation and permeability increases serving as fluid conduits.
7	Disturbed Rock Zone (DRZ)	Describes a stress-induced fracture zone around excavations in halite and anhydrite with elevated permeability and porosity that evolves over time.
8	Actinide Transport in the Salado	Assumes dissolved actinides are advected only through interbeds (modeled as porous media) while neglecting sorption and diffusion in intact halite.
9	Units Above the Salado	Defines the hydrogeologic properties of Rustler Formation units, treating only the Culebra as hydraulically significant for radionuclide release.
10	Transport of Dissolved Actinides in the Culebra	Uses a double-porosity framework with advection, dispersion, matrix diffusion, and sorption (Kd) in the rock matrix to simulate dissolved actinide transport.
11	Transport of Colloidal Actinides in the Culebra	Classifies colloids by size (intrinsic, humics, microbes, mineral fragments) and models their advection, diffusion, and filtration in the Culebra.
12	Exploration Boreholes	Characterizes inadvertent deep drilling holes that penetrate waste panels, their casing and plugging scenarios, degradation over time, and fluid flow pathways.
13	Cuttings and Cavings	Calculates volumes of waste particles brought to the surface as drill cuttings and eroded cavings based on drill-bit diameter, rock shear resistance, and drilling fluid properties.

	Conceptual Model	Summary ‡
14	Spallings	Models particulate release when repository gas pressure exceeds mud hydrostatic pressure during drilling, entraining waste as the gas blows out the borehole.
15	Direct Brine Release*	Simulates transient brine flow to the surface in drilling intrusions when repository pressure exceeds the hydrostatic pressure of the mud column and local saturation is above residual.
16	Castile Formation and Brine Reservoir	Treats the Castile Formation as impermeable except for discrete brine reservoirs with specified pressure, porosity, compressibility, and limited connectivity unless a borehole intersects them.
17	Multiple Intrusions	Extends the single-borehole intrusion model to sequences of E1 (with brine reservoir) and E2 (without) intrusions in the same panel, mapping each sequence to one of three disturbed performance scenarios.
18	Climate Change	Evaluates the effects of plausible future climate-driven recharge variations on regional groundwater flow by scaling Culebra flow fields in performance assessment.
19	Creep Closure	Represents time-dependent closure of rooms and drifts by salt creep and waste consolidation, coupled to gas and brine pressure evolution.
20	Shafts and Shaft Seals	Simplifies the four WIPP shafts into one shaft with discrete seal component regions whose effective permeabilities evolve over time to simulate sealing performance and DRZ healing.
21	Gas Generation	Accounts for repository gas production from anoxic corrosion of metals, microbial degradation of cellulosics, plastics, and rubbers and brine radiolysis as a function of brine availability.
22	Chemical Conditions	Assumes MgO backfill buffers pH (9–10) and CO_2 fugacity; fixes brine chemistry, ligand inventories, and redox conditions; and applies instantaneous thermodynamic equilibrium for solubility calculations.
23	Dissolved Actinide Source Term	Determines maximum dissolved concentrations of Th, U, Np, Pu, Am, and Cm using solubility limits for assumed oxidation states under buffered repository conditions.
24	Colloidal Actinide Source Term	Quantifies actinide loadings on mobile colloidal carriers (microbes, humics, intrinsic polymers, mineral fragments) based on empirical partitioning or binding-density relationships.

* Conceptual model modified, and peer reviewed for the CRA-2026

‡ See McCormick et al. (2024) for complete descriptions.

23.3.2.1 Description of Scenarios

Scenarios for the CRA-2026 PA were the same as those used in CRA-2019 (U.S. DOE 2019) and previous applications. These scenarios were identified by considering combinations of occurrence and nonoccurrence for all potentially disruptive events (U.S. DOE 1996, Appendix PA, Section PA-2.3.2).

23.3.3 Changes or New Information for the CRA-2019 DPA

For the CRA-2019 DPA, the WIPP FEPs were reassessed to identify those that remain applicable to the disposal system and determine appropriate changes. Of the 245 WIPP FEPs considered, 161 did not change, 84 required updates to the descriptions and/or screening arguments, and 4 had their screening decisions changed for the CRA-2019 DPA (U.S. DOE 2019, Appendix SCR, Section SCR-3.0). The changes to FEP screening did not affect the conceptual models or scenarios. The conceptual models and scenarios used for the CRA-2019 DPA remained unchanged from those used in the CRA-2014 PA. The EPA found the information documenting the DOE's FEPs reevaluation process for the CRA-2019 DPA to be generally complete (U.S. EPA 2022, page 26).

23.3.4 Changes or New Information Since the CRA-2019 DPA

Since the CRA-2019 DPA, a reassessment of FEPs was performed and documented in Kirkes and McCormick (2023). Since this analysis, additional assessments of the FEPs baseline have occurred in support of the RPPCR (Kirkes 2023) and for this CRA-2026 (McCormick and Kirkes 2025). While many FEPs have been updated as a result of these assessments, no new FEPs have been screened into PA calculations. Updates to FEPs are summarized in Table SCR-1 of Appendix SCR-2026. Due to the addition of replacement panels 11 and 12 and associated mains and drifts into the PA model, the implementation of the Disposal System Geometry, Repository Fluid Flow, and Direct Brine Release conceptual models were modified. Although the models themselves were not altered, the modified implementations of these conceptual models were incorporated into the Additional Panels Performance Assessment (APPA), peer reviewed in 2021, and found to be adequate (Falta et al. 2021).

For the CRA-2026, the scenarios are the same as in the Compliance Certification Application (CCA). The DOE continues to demonstrate compliance with section 194.23(a)(1).

23.4 40 CFR 194.23(a)(2)

23.4.1 Background

Title 40 CFR § 194.23(a)(2) requires a description of plausible, alternative conceptual models that were considered but not used for portraying disposal system performance. It also requires an explanation for not using these models.

To meet the requirements of section 194.23(a)(2), in the CCA the DOE described the plausible alternative conceptual models considered but not used and explained why these models were not used (U.S. DOE 1996, Chapters 2.0, 9.0, and Appendix MASS). In the peer reviews for conceptual model updates for the CRA-2004 and CRA-2009, alternative conceptual models were considered by the peer review panels.

23.4.2 Changes or New Information for the CRA-2019 DPA

The conceptual models used in the CRA-2019 DPA were not changed from those used in the CRA-2009 Performance Assessment Baseline Calculation (U.S. DOE 2009). With the CRA-2019 DPA an alternative PA model, called CRA19_CL, was executed where the open areas were modeled as less permeable and more isolating (Zeitler et al. 2019).

23.4.3 Changes or New Information Since the CRA-2019 DPA

For the CRA-2026, three conceptual models (Disposal System Geometry, Repository Fluid Flow, and Direct Brine Release) were subjected to a new peer review. Alternative implementations of these models were evaluated and presented to the peer review panel. These alternative implementations included a three-dimensional fluid flow model of the disposal system, and a direct brine release model that conserved the entire waste area volume. The reasons given for not using these alternative implementations models were examined by the peer review panel. The peer review panel found the approach used in the APPA to be reasonable and acceptable (Falta et al. 2021). Thus, the DOE continues to demonstrate compliance with section 194.23(a)(2).

23.5 40 CFR 194.23(a)(3)

23.5.1 Background

Title 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:

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

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

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

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

v. Peer review in accordance with section 194.27 has been conducted on the conceptual models.

23.5.2 Documentation

A description of WIPP PA code documentation is given here to assure completeness and accuracy. Documentation includes:

- User's Manual (UM)— A document intended to guide the software user. The UM contains, as applicable, the software name and version identifier; the platform(s); a statement of functional limitations; instructions that describe the user's interaction with the software; the identification and description of input and output specifications and formats; the valid ranges of input data; guidance for interpreting, debugging, error messages, and user responses; a description of any required training necessary to use the software; and an explanation of the mathematical model(s).

- Analysis Packages (APs)—A document containing detailed information on how the computer codes were used in the PA, including code implementation approaches and justification of parameters used. Each code supplies the following information relevant to section 194.23(c)(1) in its APs:

    - A 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 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.

There are five additional documents as secondary references:

- Requirements Document (RD)— A software document that contains the requirements that the product must satisfy, including functionality, design constraints, attributes (including acceptance criteria), and external features.

- Verification and Validation Plan (VVP)— A software document that delineates the test processes and associated acceptance criteria to be performed during the validation phase.

- Design Document (DD)— A document that describes the major features of the software design: theoretical basis, embodied mathematical model, control flow, control logic,

data structure(s), 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)— A document that contains the source code listing (the source code can be stored in a configuration management tool) and documentation of the process used to convert the source code to an executable.

- Validation Document (VD)— A software document that contains the results of the performance verification and validation tests defined in the VVP and evaluation of the outputs of those tests to demonstrate that the software produces valid results for problems encompassing the range of permitted usage as defined by the UM.

23.5.3 Changes or New Information for the CRA-2019 DPA

23.5.3.1 Conceptual Models

All conceptual models used in the CRA-2019 DPA were previously peer reviewed. No modifications were made to the conceptual models from the CRA-2009 PA to the CRA-2019 DPA. The EPA found that the DOE complied with section 194.23(a)(3)(i) for the CRA-2019 (U.S. EPA 2022, page 27).

23.5.3.2 Mathematical Models

No changes were made in the methodology used to document mathematical models and initial and boundary conditions. Discussions of the mathematical models and initial and boundary conditions are found in Appendices PA-2019, SOTERM-2019, and GEOCHEM-2019. The UMs and APs are also used to document mathematical models and the initial and boundary conditions.

One new code, PHREEQCI version 2.12.5-669, was added to the WIPP PA calculations for the CRA-2019 DPA. While PHREEQCI was documented and qualified for use on the WIPP project in 2006, it was never used for compliance calculations until the CRA-2019 DPA. In the CRA-2019 DPA, PHREEQCI was used to calculate the humic colloid parameter values.

Two codes, BRAGFLO and PANEL, had significant modifications for the CRA-2019 DPA. Due to hardware upgrades, most other PA codes saw minor updates for the CRA-2019 DPA.

In their review of the CRA-2019, the EPA found that the “DOE continues to adequately document and describe simplifications of conceptual models in the CRA-2019 PA and continues to provide an adequate technical basis to support the mathematical formulations” (U.S. EPA 2022, page 27).

23.5.3.3 Numerical Models

As in the CRA-2014 PA calculations, the information used to evaluate the stability of numerical schemes was provided in the VDs and APs prepared for each of the CRA-2019 DPA computer codes. The EPA found that the DOE continued to adequately set the range of functional tests for each code to verify that the code performs as expected and provides reasonable results (U.S. EPA 2022, page 27).

23.5.3.4 Computer Codes

For CRA-2019 DPA, the same four-phase computer code development process used in CRA-2014 was used—requirements, design, implementation, and software verification and validation—ensuring the codes remained error-free, stable, and accurately implemented numerical models. Information documenting code development and requirements is contained in the RD, VVP, VD, and ID prepared for each code used in the CRA-2019 DPA calculations.

The EPA determined that the CRA-2019 PA computer codes continued to comply with section 194.23(a)(3)(iv) (U.S. EPA 2022, page 27).

23.5.3.5 Peer Review

For the CRA-2019, there were no new peer reviews since the CRA-2009. The EPA determined that the DOE continued to demonstrate compliance with the provisions of section 194.23(a)(3)(v).

23.5.4 Changes or New Information Since the CRA-2019 DPA

23.5.4.1 Conceptual Models

All conceptual models used in the CRA-2026 PAs have been peer reviewed. Since the CRA-2019 DPA, three conceptual models have undergone peer review: the Disposal System Geometry, Repository Fluid Flow, and Direct Brine Release conceptual models. The peer review examined the implementation of these conceptual models as they were affected by modifications to represent replacement and proposed additional panels. The peer review panel found the conceptual models continue to be reasonable and adequate for use in WIPP PA (Falta et al. 2021). Therefore, the DOE continues to demonstrate compliance with the provisions of section 194.23(a)(3)(i).

23.5.4.2 Mathematical Models

Three new codes were introduced to the WIPP PA since the CRA-2019 DPA: MODFLOW6 (Langevin et al. 2017), PEST++ (White et al. 2020), and SIERRA_SM (SNL 2022). MODFLOW6 replaces MODFLOW2000 for modeling flow in the Culebra Dolomite Member of the Rustler Formation. PEST++ replaces PEST for optimizing the fit of transmissivity fields to data. SIERRA_SM replaces SANTOS (Stone 1997) to model creep closure of the Salado Formation and consolidation of the waste-filled repository.

Four WIPP PA codes had major revisions since the CRA-2019 DPA. The code CCDFGF, which calculates repository release distributions from Monte Carlo simulations, and its companion preprocessor PRECCDFGF were both modified to accommodate the replacement and proposed additional panels. The Latin Hypercube Sampling code, LHS, was enhanced to maintain consistent random sampling across different computing platforms. The BRAGFLO code, used to model two-phase fluid flow in and around the repository, was updated to add a modified capillary-pressure model that imposes a lower bound on capillary pressure in the anhydrite marker beds. Due to hardware upgrades, most other PA codes have had minor updates since the CRA-2019 DPA.

For the existing, updated, and new codes, documentation continues to demonstrate that mathematical models incorporate equations and boundary conditions that reasonably represent the mathematical formulation of the conceptual models. Thus, the DOE continues to demonstrate compliance with the provisions of section 194.23(a)(3)(ii).

23.5.4.3 Numerical Models

As in the CRA-2019 DPA calculations, the information used to evaluate the stability of numerical schemes is provided in the VDs and APs prepared for each CRA-2026 PA computer code. Thus, the DOE remains in compliance with the provisions of section 194.23(a)(3)(iii).

23.5.4.4 Computer Codes

To show that the PA computer codes continue to be free of coding errors, produce stable results, and implement the numerical models correctly, the same computer code development process and requirements was used for the CRA-2026 PA computer codes as was used in previous PA calculations, which consisted of four primary development phases: (1) requirements phase; (2) design phase; (3) implementation phase; and (4) software verification and validation. Information documenting code development and requirements is contained in the RD, VVP, VD, and ID prepared for each of the codes used in the CRA-2026 PA calculations. On this basis, the DOE continues to demonstrate compliance with the provisions of section 194.23(a)(3)(iv).

23.5.4.5 Peer Review

The Additional Panels Peer Review was completed in 2021 (Falta et al. 2021). The peer review panel evaluated changes to the implementation of the Disposal System Geometry, Repository Fluid Flow, and Direct Brine Release conceptual models needed for the WIPP PA to model replacement and additional panels to the west of the existing repository. The EPA observed the peer review meetings and reviewed the peer review procedures, processes, and findings. The EPA found that the peer review was conducted in accordance with the requirements of 40 CFR § 194.27 and 194.23 (a)(3)(v) (U.S. EPA 2023). Thus, the DOE continues to demonstrate compliance with the provisions of section 194.23(a)(3)(v).

23.6 40 CFR 194.23(b)

23.6.1 Background

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

23.6.2 Changes or New Information for the CRA-2019 DPA

The computer code quality assurance program did not change for the CRA-2019 DPA. To demonstrate that computer software complies with disposal regulations, software used to support the PA used the established life-cycle management process. The software qualification approach follows the life-cycle phases outlined in the American Society of Mechanical Engineers (ASME) Nuclear Quality Assurance (NQA)-2a-1990 addendum, part 2.7. The EPA determined that the DOE continued to comply with the requirements for section 194.23(b) for CRA-2019 (U.S. EPA 2022, page 27).

23.6.3 Changes or New Information Since the CRA-2019 DPA

The computer code quality assurance program has not changed for the CRA-2026. This program follows a life-cycle management process for software as outlined in the ASME NQA-2a-1990 addendum, part 2.7. Thus, the DOE continues to comply with the requirements for section 194.23(b).

23.7 40 CFR 194.23(c)(1)

23.7.1 Background

Title 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.

Descriptions of the theoretical backgrounds of each model and the method of analysis or assessment were primarily contained in DD, UM, RD, VVP, ID, and VD for each code.

23.7.2 Changes or New Information for the CRA-2019 DPA

No changes were made to the documentation procedure of PA computer codes used in the CRA-2019 DPA.

The EPA found that the DOE's level of documentation continued to be adequate and consistent with the level of documentation produced previously. The EPA concluded the DOE continued to be in compliance with section 194.23(c)(1) for CRA-2019 (U.S. EPA 2022, page 28).

23.7.3 Changes or New Information Since the CRA-2019 DPA

No changes have been made to the documentation procedures for PA computer codes used in the CRA-2026. In CRA-2026, the information is primarily contained in the DD, UM, RD, VVP, ID, and VD for each code. Thus, the DOE continues to demonstrate compliance with the provisions of section 194.23(c)(1).

23.8 40 CFR 194.23(c)(2)

23.8.1 Background

Title 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 quality assurance procedures.

Documentation required by section 194.23(c)(2) is primarily contained in the UM, AP, RD, VVP, ID, and VD for each code.

23.8.2 Changes or New Information for the CRA-2019 DPA

No changes were made to the documentation procedures for PA computer codes used in the CRA-2019 DPA.

23.8.3 Changes or New Information Since the CRA-2019 DPA

No changes were made to the documentation procedures for PA computer codes used in the CRA-2026 PAs. Documentation required by section 194.23(c)(2) is primarily contained in the UM, AP, RD, VVP, ID, and VD for each code. Thus, the DOE continues to demonstrate compliance with the provisions of section 194.23(c)(2).

23.9 40 CFR 194.23(c)(3)

23.9.1 Background

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

23.9.2 Changes or New Information for the CRA-2019 DPA

The information relevant to compliance with section 194.23(c)(3) is contained in the ID for each modeling code.

23.9.3 Changes or New Information Since the CRA-2019 DPA

The information relevant to compliance with section 194.23(c)(3) is contained in the ID for each modeling code. Thus, the DOE continues to demonstrate compliance with the provisions of section 194.23(c)(3).

23.10 40 CFR 194.23(c)(4)

23.10.1 Background

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

23.10.2 Changes or New Information for the CRA-2019 DPA

There were no changes to the process for documenting parameters for the CRA-2019 DPA. Since the CRA-2014, there were 64 parameter updates, and 42 new parameters defined for analyses performed between the CRA-2014 and the CRA-2019 DPA, including parameters added for the CRA14_SEN2, CRA14_SEN3, CRA14_SEN4, and APCS analyses. These parameters were needed for model updates, including changes to modeling the DRZ over time and the representation of abandoned panel closures. There were also 10 new parameters and 152 parameter updates for the CRA-2019 DPA, most of which were inventory and drilling parameter updates (Kim and Feng 2019, Table 2). The EPA reviewed the new and updated parameters in the CRA-2019 DPA. The EPA determined the DOE continued to comply with section 194.23(c)(4) for the CRA-2019 (U.S. EPA 2022, page 28).

23.10.3 Changes or New Information Since the CRA-2019 DPA

There were no changes to the process for documenting new parameters or updating parameter values since the CRA-2019 DPA. In the CRA-2026 there are 21 new parameters for the oxidation-state model, iron surface area calculation for iron corrosion, early-time gas generation from cellulose, plastic, and rubber biodegradation, and microbial colloids. There are 157 updated parameters in the CRA-2026, most of which are related to inventory and drilling information updates (Feng and Kicker 2025, Table 2). Thus, the DOE continues to comply with section 194.23(c)(4).

23.11 40 CFR 194.23(c)(5)

23.11.1 Background

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

No licenses from software vendors have been required to operate the codes essential for the WIPP PA. Most computer codes for the WIPP PA were developed by Sandia National

Laboratories (SNL) as custom software and require no licenses to execute. Other acquired codes have been in the public domain and readily accessible.

23.11.2 Changes or New Information for the CRA-2019 DPA

The new code added for the CRA-2019 DPA, PHREEQCI, is open source and freely available from the U.S. Geological Survey. No other changes to software licenses for codes used in the WIPP PA were made. The EPA determined the DOE complied with section 194.23(c)(5) (U.S. EPA 2022, page 28).

23.11.3 Changes or New Information Since the CRA-2019 DPA

The new code SIERRA_SM is export-controlled under U.S. Department of Commerce Export Regulations and U.S. State Department Regulations. The SIERRA_SM executable used for the WIPP PA room porosity calculation is available on the SNL WIPP PA computing cluster.

The new codes MODFLOW6 and PEST++ are in the public domain and the source codes are freely available from the U.S. Geological Survey. Thus, the DOE continues to demonstrate compliance with section 194.23(c)(5).

23.12 40 CFR 194.23(c)(6)

23.12.1 Background

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

23.12.2 Changes or New Information for the CRA-2019 DPA

Parameter correlations used in the CRA-2019 DPA were documented in Kim and Feng (2019, section 4.0). The EPA determined that the DOE complied with section 194.23(c)(6) (U.S. EPA 2022, page 28).

23.12.3 Changes or New Information Since the CRA-2019 DPA

Parameter correlations used in the CRA-2026 are documented in Feng and Kicker (2025, section 4.0). No changes have been made in parameter correlations since the CRA-2019 DPA. Thus, the DOE continues to demonstrate compliance with section 194.23(c)(6).

23.13 40 CFR 194.23(d)

23.13.1 Background

Title 40 CFR § 194.23(d) requires the DOE to provide the EPA, on request, access to data files, source codes, executables, computing hardware, and other information necessary to perform independent simulations.

23.13.2 Changes or New Information for the CRA-2019 DPA

During the EPA's review of the CRA-2019 DPA, the EPA was provided with access to the SNL computing cluster where the WIPP PA calculations are performed. The EPA determined that the DOE complied with section 194.23(d) for the CRA-2019 (U.S. EPA 2022, page 30).

23.13.3 Changes or New Information Since the CRA-2019 DPA

In compliance with section 194.23(d), access to the computer hardware and software needed to perform independent simulations will continue to be provided to the EPA. The new code SIERRA_SM is export controlled under U.S. Department of Commerce Export Regulations and State Department Regulations. The SIERRA_SM executable used for the WIPP PA room porosity calculation is available on the SNL WIPP PA computing cluster. Thus, the DOE continues to demonstrate compliance with the provisions of section 194.23(d).

23.14 References

(*Indicates a reference that has not been previously submitted.)

Falta, R., M. Hu, E. M. Kwicklis, C. I. Steefel, S. C. Williams-Stroud, and J. A. Thies. 2021. Additional Panels Performance Assessment (APPA) Changed Conceptual Models Peer Review Report. Carlsbad, NM: U.S. Department of Energy, Carlsbad Field Office. *

Feng, L. and D. Kicker. 2025. Input Parameter Report for the 2026 Compliance Recertification Application Performance Assessment: Interim State Repository (CRA-2026 IS). Revision 1. Carlsbad, NM: Sandia National Laboratories. *

Kim, S. and L. Feng. 2019. Input parameter report for the 2019 Compliance Recertification Application Performance Assessment (CRA-2019 PA) Revision 1. Carlsbad, NM: Sandia National Laboratories. ERMS 571660.

Kirkes, G. R. 2023. Features, Events, and Processes Analysis for the Replacement Panels Planned Change Request Performance Assessment. Carlsbad, NM: Sandia National Laboratories. ERMS 579720. *

Kirkes, G. R. and J. McCormick. 2023. Analysis Report for the Reassessment of Features, Events, and Processes Analysis for the 2024 Compliance Recertification Application. Carlsbad, NM: Sandia National Laboratories. ERMS 580866. *

Langevin, C.D., J.D Hughes, E.R. Banta, R.G. Niswonger, S. Panday, and A.M. Provost. 2017. Documentation for the MODFLOW 6 Groundwater Flow Model: U.S. Geological Survey Techniques and Methods, Book 6, Chap. A55, p. 197. ERMS 577793. *

McCormick, J., R. Kirkes, and C. Hansen. 2024. Conceptual Models in WIPP Performance Assessment. October 8, 2024. Carlsbad, NM: Sandia National Laboratories. EIMS-0004385596. *

McCormick, J. and R. Kirkes. 2025. Features, Events, and Processes Assessment for the Compliance Recertification Application - 2026, Revision 0. Carlsbad, NM: Sandia National Laboratories. EIMS- 0004940580 *

Sandia National Laboratories (SNL). 2022. Sierra Solid Mechanics 5.4 User's Guide. Albuquerque, NM: Sandia National Laboratories. SAND2022-0103. *

Stone, C.M. 1997. SANTOS—A Two-Dimensional Finite Element Program for the Quasistatic, Large Deformation, Inelastic Response of Solids. Albuquerque, NM: Sandia national Laboratories. SAND90-0543

U.S. Department of Energy (DOE). 1996. Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant (October). Carlsbad, NM: Carlsbad Field Office. DOE/CAO 1996-2184.

U.S. DOE. 2009. Title 40 CFR Part 191 Compliance Recertification Application for the Waste Isolation Pilot Plant (March). Carlsbad, NM: Carlsbad Field Office. DOE/WIPP 2009-3424.

U.S. DOE 2019. Title 40 CFR Part 191 Compliance Recertification Application for the Waste Isolation Pilot Plant. Carlsbad, NM: Carlsbad Field Office. DOE/WIPP 19-3609.

U.S. Environmental Protection Agency (EPA). 1993. 40 CFR Part 191 Environmental Radiation Protection Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes: Final Rule. *Federal Register,* vol. 58 (December 20, 1993): 66398–416.

U.S. EPA. 1996. 40 CFR Part 194: Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance with the 40 CFR Part 191 Disposal Regulations; Final Rule. *Federal Register*, vol. 61 (February 9, 1996): 5223–5245.

U.S. EPA. 2022. 2019 Compliance Recertification Application Review Document (CARD). 40 CFR §§ 191 & 194. Washington, DC: Office of Radiation and Indoor Air (April 2022). EPA-HQ-OAR-2019-0534. *

U.S. EPA. 2023. EPA Review of DOE Peer Review of Conceptual Changes Incorporated in the APPA Model. Washington, DC: Office of Radiation and Indoor Air (April 2023). EPA-HQ-OAR-2001-0012-0774. *

White, J., R. Hunt, M. Fienen, and J. Doherty. 2020. Approaches to Highly Parameterized Inversion: PEST++ Version 5, a Software Suite for Parameter Estimation, Uncertainty Analysis,

Management Optimization and Sensitivity Analysis: U.S. Geological Survey Techniques and Methods 7C26, 52 p. *

Zeitler, T. R., J. Bethune, S. Brunell, B. Day, D. Kicker, J. Long, and R. Sarathi. 2019. Summary Report for the 2019 Compliance Recertification Application Performance Assessment (CRA-2019 PA). 2019. Carlsbad, NM: Sandia National Laboratories. ERMS 571376