JUN 24 1998

SAND--98-0180/1

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SAND98–0180/1
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# Guidebook for Performance Assessment Parameters Used in the Waste Isolation Pilot Plant Compliance Certification Application

## Volume I: Main Report

Susan M. Howarth, Mary-Alena Martell, Ruth Weiner, Charlene Lattier

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# Guidebook for Performance Assessment Parameters Used in the Waste Isolation Pilot Plant Compliance Certification Application

## Volume I: Main Report

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## ABSTRACT

The Waste Isolation Pilot Plant (WIPP) Compliance Certification Application (CCA) Performance Assessment (PA) Parameter Database and its ties to supporting information evolved over the course of two years. When the CCA was submitted to the Environmental Protection Agency (EPA) in October 1996, information such as identification of parameter value or distribution source was documented using processes established by Sandia National Laboratories WIPP Quality Assurance Procedures. Reviewers later requested additional supporting documentation, links to supporting information, and/or clarification for many parameters. This guidebook is designed to document a pathway through the complex parameter process and help delineate flow paths to supporting information for all WIPP CCA parameters. In addition, this report is an aid for understanding how model parameters used in the WIPP CCA were developed and qualified. To trace the source information for a particular parameter, a dual-route system was established. The first route uses information from the Parameter Records Package as it existed when the CCA calculations were run. The second route leads from the EPA Parameter Database to additional supporting information.

**ACKNOWLEDGMENTS**

The authors thank the other members of the CCA Parameter Team: Lori Dotson and Deborah Coffey, Karen Schmeige (SAIC), and J.T. Schneider and Gretchen Newman (GRAM, Inc.) for their help during the parameter development process and subsequent CCA parameter reviews and audits. Their feedback provided the framework for this guidebook.

The authors also thank Lori Dotson, Diane Hurtado, and Martin Tierney for their helpful review comments and Carol Crawford for her thorough reference and literature review. In addition, the authors thank Tim Peterson (Tech Reps, Inc.) for his help in shaping this document into final form.

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## Nomenclature

| | |
|---|---|
| 1992 PA | WIPP Performance Assessment calculation performed in 1992 |
| a.m.u. | atomic mass unit |
| ASME | American Society of Mechanical Engineers |
| BIR | (WIPP) Baseline Inventory Report |
| CAO | Carlsbad Area Office (of the DOE) |
| CCA | Compliance Certification Application (DOE, 1996) |
| CCDF | Complementary Cumulative Distribution Function |
| CDB | Computational Database |
| CFR | Code of Federal Regulations |
| CH-TRU | Contact-Handled TRU |
| CMS | Configuration Management System |
| DBA | Database Administrator |
| DEC | Digital Equipment Corporation |
| DOE | United States Department of Energy |
| E.D.T.A. | Ethelyne diamine tetra-acetate |
| EPA | Environmental Protection Agency |
| FEP | Features, Events, and Processes |
| IRT | Independent Review Team |
| LANL | Los Alamos National Laboratory |
| LHS | Latin hypercube sampling |
| NAS | National Academy of Sciences |
| NQA | Nuclear Quality Assurance |
| NUREG | Nuclear Regulatory Commission Regulatory Guide |
| ORNL | Oak Ridge National Laboratory |
| PA | Performance Assessment |
| PAA | Performance Assessment Analyst |
| PAR | Appendix PAR of the CCA (DOE, 1996) |
| PI | Principal Investigator |
| PIPP | Principal Investigator Parameter Package |
| PRP | Parameter Records Package |

## Nomenclature (concluded)

| | |
|---|---|
| PTL | Parameter Task Leader |
| QA | Quality Assurance |
| QAP | SNL WIPP Quality Assurance Procedure |
| QAPD | Quality Assurance Program Document (CAO) |
| QAPD | Quality Assurance Program Description (SNL WIPP) |
| QED | Qualification of Existing Data |
| RH-TRU | Remote-Handled TRU |
| SNL | Sandia National Laboratories |
| SRS | Savannah River Site |
| SWCF | Sandia WIPP Central Files |
| TRU | transuranic |
| TWBIR | Transuranic Waste Baseline Inventory Report |
| UNIX | Trade name of AT&T computer operating system |
| VAX | Trade name of DEC computer hardware |
| WID | Westinghouse Electric Corporation Waste Isolation Division |
| WIPP | Waste Isolation Pilot Plant |
| WPO number | WIPP Project Office file code number for documents filed in the SWCF |

# 1. Introduction

The Waste Isolation Pilot Plant (WIPP) Compliance Certification Application (CCA) Performance Assessment (PA) Parameter Database and its ties to supporting information evolved as the work of the code sponsors, parameter task leaders, performance assessment analysts, experimental principal investigators, and quality assurance (QA) personnel was integrated over the course of two years. When the CCA (DOE, 1996) was submitted in October 1996, information such as identification of parameter value or distribution source was documented using processes established by Sandia National Laboratories (SNL) WIPP Quality Assurance Procedures (QAPs).

After submitting the CCA, Environmental Protection Agency (EPA) staff, QA auditors, SNL technical staff, and others reviewing the parameters and supporting information requested ties to supporting information, additional supporting documentation, and/or clarification for many parameters. The additional supporting information was documented in memoranda and in a database (*wipp_reference*) created specifically for post-CCA submittal reviews from the WIPP CCA PA Parameter Database. The *wipp_reference* database, referred to here as the EPA Parameter Database, and the memoranda were filed in the Sandia WIPP Central Files (SWCF) with the original supporting information. The trail from the parameter distributions used in the CCA database to supporting information has become very complex as a result.

This guidebook was designed to fully document a pathway through the complex parameter process and help delineate flow paths to supporting information for all WIPP CCA parameters. In addition, it was designed as an aid for understanding how model parameters used in the WIPP CCA were developed and qualified. Section 2 of this report contains details regarding parameter definition and identification. Section 3 contains information regarding the qualification of the parameters and the supporting data or other information. Section 4 delineates the parameter development process; roles and responsibilities are discussed as well as the formal and informal processes used to develop and document the parameters. Section 5 contains information about the relational database that contains the parameter information used for the 1996 CCA Calculations. Sections 6 contains detailed information about WIPP Data Entry Form 464. Section 7 discusses parameter traceability and retrieveability using the Parameter Records Package (PRP) system and the EPA Parameter Database. References are contained in Section 8.

Ideally, users would be able to trace from the parameter information contained in the WIPP PA Parameter Database to supporting information using only the information contained in the PRP. However, as described in Section 7, in order to trace through to the source information for a particular parameter, two routes should be followed. The first route uses information contained or referenced in the PRP as it existed when the CCA calculations were run. The second route leads from the EPA Parameter Database to additional supporting information. For completeness, users should follow both paths to properly reach and review the information supporting a particular parameter.

## 1.1 Records

Two copies of all parameter-related records (and other WIPP records) are stored in the SWCF in Albuquerque, NM. Documents are assigned WIPP Project Office (WPO) numbers by SWCF staff. When requesting a document from the SWCF, it is helpful to know its WPO number or its author, date, and title.

Page intentionally blank

# 2. Parameters

## 2.1 Definition

For the purposes of the CCA PA, a parameter is defined as any number needed to implement the WIPP CCA PA codes. Parameter distribution values are developed based on data, literature, technical references, and other source information.

## 2.2 Identification

Each parameter in the CCA PA Parameter Database is uniquely identified in WIPP documentation one of three ways: by either (1) its id number, (2) its two-part name consisting of its material name (idmtrl) and its property name (idpram), or (3) the WPO number of its PRP. For example, the Castile Brine Reservoir rock compressibility parameter is identified by its assigned id number (61), its two-part name (CASTILER:COMP_RCK), or by the WPO number of its PRP (31561). In this example, CASTILER is the idmtrl alphanumeric for the material name, Castile Brine Reservoir; COMP_RCK is the idpram alphanumeric for the property name, rock compressibility.

The alphanumeric identifiers for the waste chemistry parameters were derived as follows: Chemistry parameters associated with dissolved actinides are identified with a material name (idmtrl) that is either the chemical symbol for the radionuclide or isotope (e.g., AM, PU, AM241, PU238), the oxidation or valence state of the radionuclide or isotope (e.g., AM+3, PU+4), or the solubility of the radionuclide or valence state (e.g., SOLAM3, SOLMOD6). The property name for dissolved actinides denotes the chemical conditions (e.g., SILCIM for Castile brine, inorganic environment, MgO present) or, for retardation, the distribution coefficient (e.g., MKD_PU).

For the chemistry parameters associated with colloids, the material name (idmtrl) is the chemical symbol for the radionuclide (i.e., AM, PU), or it incorporates the valence state (e.g., PHUMOX4: the proportion of actinides sorbed on humic colloids in valence states +4). The property name (idpram) for colloids indicates either the chemical conditions (e.g., PHUCMIM) or the type of colloid and the amount of actinides sorbed (e.g., CONCMIN: the actinide concentration on mineral fragment colloids; CAPHUM: the maximum actinide concentration [cap] on humic colloids; PROPMIC: the proportion of actinides sorbed on microbial colloids).

Appendices A1 and A2 contain the dictionaries that describe the materials and properties idmtrl and idpram, respectively. Figures 1 and 2 illustrate the grid forms used in the CCA for the undisturbed and disturbed WIPP scenarios, respectively. Each number on Figures 1 and 2 corresponds to a table contained in Appendix A3 that associates parameters to materials in that section of the grid (see Table 1).

The tables of parameters contained in Appendix A3 are keyed to the materials to which the parameters are assigned. The tables contain the parameter identification alphanumerics, dimension (units) of each parameter, distribution type, range of values for each parameter, category, code using the parameter, and WPO number for the PRP for the particular parameter. Note that Table 31 of Appendix A3 contains global parameters (i.e., parameters that can be associated with any area of the grid). Table 32 of Appendix A3 contains reference constants that are not associated with a specific area of the grid (e.g., gravitational constant and *pi*). The tables that associate the WIPP Baseline Inventory Report (BIR) (DOE, 1995-1996) waste chemistry to the waste panels were subdivided into four tables (Tables 23B, C, D, and E of Appendix A3) for convenience.

Appendices B1, B2, and B3 are provided as a lookup table to assist readers in identifying specific parameters: Appendix B1 lists parameters sorted by id number; Appendix B2 lists parameters sorted by material name, and Appendix B3 lists parameters sorted by property name.

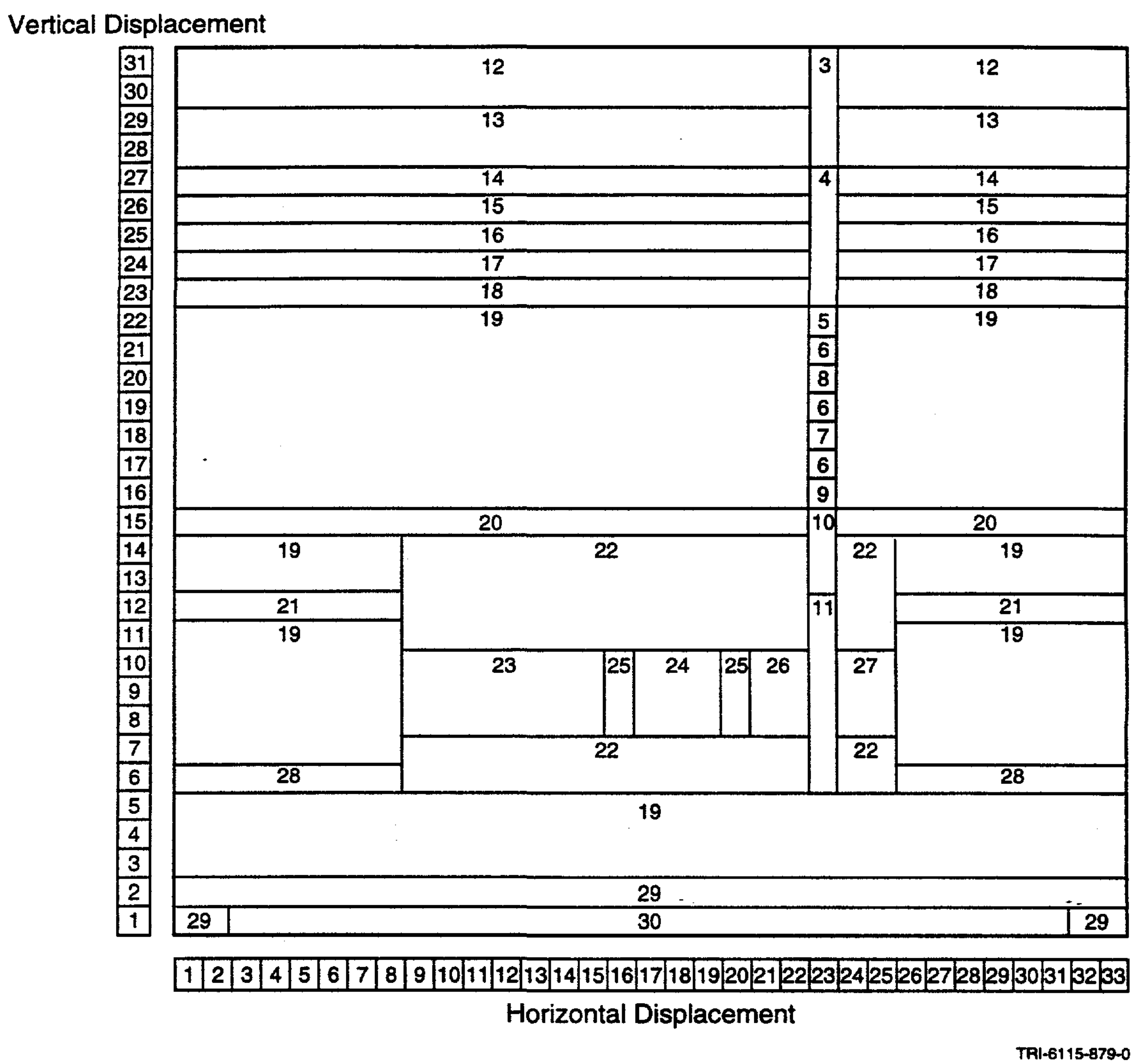


Figure 1. Grid form for undisturbed scenario.

## 2.3 Sampled Parameters

Appendix PAR of the CCA (DOE, 1996) contains details regarding the parameters that were sampled by the Latin hypercube sampling (LHS) code during the CCA PA calculations. A listing of these sampled parameters is included in Appendix H for convenience. Further discussion of the LHS and probabilistic analyses are found in Section 6.1.5 of the CCA (DOE, 1996).

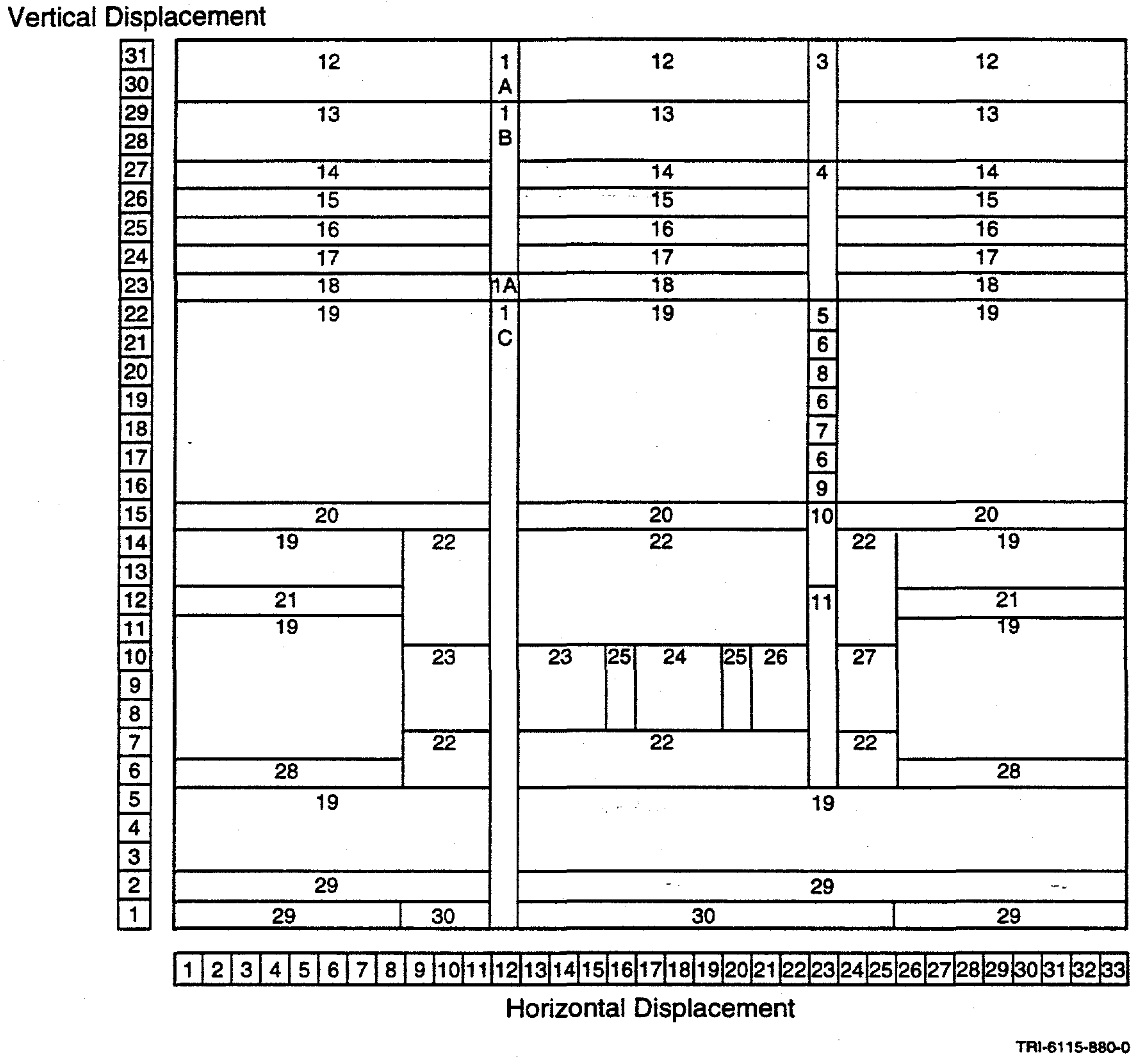


Figure 2. Grid form for disturbed scenario.

Table 1. Grid Form Number and Cross Reference to Material Tables in Appendix A3

| Grid Form/Appendix A-3 Table Number | Material |
|---|---|
| 1 | Borehole, Blowout, Drillmud |
| 1A | Borehole Concrete Plug |
| 1B | Borehole Open |
| 1C | Borehole Silty Sand |
| 1D | Borehole Creep |
| 2 | Shaft Disturbed Rock Zone |
| 3 | Earthen Fill |
| 4 | Rustler Compacted Clay |
| 5 | Asphalt |
| 6 | Shaft Concrete |
| 7 | Shaft Crushed Salt (time periods 1–6) |
| 8 | Upper Shaft Clay (time periods 1–5) |
| 9 | Lower Shaft Clay (time periods 1–4) |
| 10 | Bottom Clay Component |
| 11 | Concrete Monolith |
| 12 | Santa Rosa Formation |
| 13 | Dewey Lake Red Beds |
| 14 | Forty Niner Member |
| 15 | Magenta Dolomite |
| 16 | Tamarisk Member |
| 17 | Culebra Dolomite |
| 18 | Unnamed Lower Member |
| 19A | Salado Halite |
| 19B | Salado Brine |
| 20 | Marker Bed 138 |
| 21 | Anhydrite Beds A&B |
| 22 | Disturbed Rock Zone |
| 23A | Waste Panel |
| 23B | Waste Chemistry |
| 24A | Rest of Repository |
| 24B | Predisposal Cavities |
| 25 | Panel Closure |
| 26 | Operations Region |
| 27 | Experimental Area |
| 28 | Marker Bed 139 |
| 29 | Castile Formation |
| 30A | Castile Reservoir |
| 30B | Castile Brine |
| 31 | Global |
| 32 | Reference Constants |

# 3. Qualification

This section describes the qualification basis for data and parameters developed and used in support of the WIPP CCA. As described in this section, all data used in the development of parameters for the WIPP CCA calculations were qualified and considered to be valid data, just as all parameters used in the WIPP CCA were qualified and considered to be valid parameters.

## 3.1 Data Qualification

As described in Chapter 5 of the CCA, data supporting a parameter are qualified if

1. the data were part of a peer review process or compared to corroborating data or substantiated by the results of confirmatory testing using a process consistent with the requirements of 40 CFR Part 194; or
2. the data were developed under the approved SNL QA program or developed under an approved SNL subcontractor's QA program; or
3. the data were developed under a QA program found to be equivalent under the qualification of existing data (QED) process described in SNL QAP 20-3, "Qualification of Existing Data"; or
4. the data were developed by the Westinghouse Waste Isolation Division under its approved QA program; or
5. the data are generally or historically accepted by the scientific and engineering community.

For parameters that were developed using multiple data sets or sources, multiple data qualification processes may have been used.

According to the CCA, for data qualified by approval and implementation of a QA program meeting the requirements of 40 CFR Part 194, the supporting documents include the QA plan, audit and surveillance reports of the work that produced the data, and other objective evidence of QA program implementation. If audit reports identify significant deficiencies, then data whose quality is affected by those deficiencies are not qualified until corrective actions have been implemented and verified.

For data collected prior to the DOE approval of the overall SNL QA program, another process was used to qualify data. A qualification date (T=0) is documented in summary reports that provide rationale and pointers to supporting information. For new and existing data (i.e., work completed prior to 1992), the QED process described in SNL QAP 20-3 was used to qualify the data by determining whether the QA program in effect met the requirements of 40 CFR Part 194.

Data collected by SNL and its subcontractors to support compliance were used if the data were

- collected after August 1, 1995, when the SNL QA program was approved by the DOE,
- collected after the approval of a subcontractor QA program by SNL,
- qualified by an Independent Review Team (IRT), or
- qualified by the peer review process.

Data that did not fall into one of these four categories were not used in the CCA calculations.

### 3.1.1 Qualification of Existing Data

Existing data are those data collected prior to the implementation of a QA program. Existing data, used as input to computer codes that support conceptual models, have been used to support the development of parameter values and distributions used in the performance assessment calculations. SNL QAP 9-2, "Quality Assurance Requirements for the Selection and Documentation of Parameter Values Used in WIPP Performance Assessment," describes the process for selecting parameter values used in performance assessment. To ensure that data are used as intended, the Principal Investigator (PI), the Performance Assessment Analyst (PAA), and the Parameter Task Leader (PTL) sign Form 464 (WIPP Parameter Entry Form), indicating concurrence that the proposed parameter is appropriate and the supporting documentation is sufficient. To qualify existing data to support the compliance application, a process following the guidelines of NUREG-1298 (Altman et al., 1988), as described in Chapter 5 of the CCA, was developed.

The QED process, as described in SNL QAP 20-3, includes three major steps. The first step identifies the packages to be qualified by identifying those data packages that support the performance assessment calculations. The second step includes provisions for the evaluation of the QA requirements and technical status of the data packages by an IRT. If the QA requirements applicable to the data package are determined to be acceptable, a third step is followed in which the data are qualified by peer review, confirmatory testing, or the use of corroborating data. Otherwise the data are not used.

The experiments reviewed by the QED process have been diverse, including the gas generation tests conducted at other national laboratories, the surface and underground hydrologic testing in the vicinity of the WIPP, the laboratory testing of salt properties, and other tests. The previous work reviewed was performed from 1984 to 1992. Each data package corresponded to a test plan or other test control document. Table 2 identifies the 14 packages reviewed by the IRT and determined to have been collected under an equivalent QA program.

Table 2. QED Data Packages Qualified by IRT (in accordance with SNL QAP 20-3)

| Review Group | Data Package |
|---|---|
| Salado Testing activities (two packages) | Salado in situ permeability |
| Creep and fracture tests | Clean and argillaceous salt |
| Salt compaction | Hydrostatic and shear consolidation |
| Corrosion | Steel |
| Microbial | Cellulosics, plastics, and rubbers |
| Borehole tests, two or more wells (six packages) | Drilling, drill stem and hydrologic testing, well development |
| Hydrogeologic characterization (two packages) | Permeability and water lever measurements |

Peer reviews are performed when necessary to verify the technical adequacy of work conducted to produce the required data and to qualify the data. The peer review process and peer reviews conducted to support data qualification are described in Chapter 9 of the CCA. All data sets not qualified by the IRT process or collected under an approved QA program were qualified by the peer review process. The QA records generated as a result of the IRT process described in SNL QAP 20-3 include the IRT Statement of Condition, composite checklist, recommendations for improvement, and qualifications and training of IRT members.

The WIPP CCA peer review process, which was led by the DOE Carlsbad Area Office (CAO), qualified parameters and data that were used in developing parameters. Appendix C contains a listing of parameters that were reviewed and found to be acceptable by peer review panels. The peer review panel documentation states that the process qualified the parameters; it does not explicitly state that data were qualified. The peer review panels reviewed parameters derived from qualified data that failed the QED process or parameters that were required because of changes in the conceptual models.

### 3.1.2 T=0 Process

The T=0 process implemented by SNL was used to determine the date when Nuclear Quality Assurance (NQA) program controls were adequate and effectively implemented for subcontractor activities performed prior to the approval of the SNL QA program. This process provides a traceable basis for determining when adequate QA controls were applied to subcontractor activities.

The process is documented in SNL QAP 20-7, "Establishing T=0 for Internal and External Experiment Activity QA Programs," and includes the following key elements:

1. The process evaluation was performed by a certified NQA-1 Lead Auditor and results are documented in a memorandum.
2. The QA requirements identified for the work (as described in the Statement of Work), the subcontractor QA program plan, and other implementing documents were reviewed.
3. The audit record, including audit responses and corrective actions, was reviewed to determine the requirements and objective evidence evaluated during the audit and the audit results.
4. The audit record and the associated documentary evidence were evaluated to determine when adequate controls on the work were effectively implemented. This evaluation included a review of any corrective actions and the associated responses, as well as verification of the corrective actions.
5. A determination was made of the date when adequate QA controls were applied to the work.

Appendix D contains the results of the T=0 process. The tables contained in this appendix identify the SNL subcontractor and contract number, the date of first qualification, and the corresponding audit number.

### 3.1.3 SNL QA Program

The SNL QA Program was developed to meet the requirements of the DOE/CAO Quality Assurance Program Document (QAPD) (CAO-94-1012, Rev. 1). This DOE document was written to address 40 CFR 194.22, Quality Assurance, and incorporates requirements from the following documents:

- American Society of Mechanical Engineers (ASME) Nuclear Quality Assurance Standard, NQA-1-1989 edition, *Quality Assurance Program Requirements for Nuclear Facilities*
- ASME NQA-2a-1990 addenda to NQA-2-1989, Part 2.7, *Quality Assurance Requirements of Computer Software for Nuclear Facility Applications*

- ASME NQA-3-1989 edition, *Quality Assurance Program Requirements for the Collection of Scientific and Technical Information for Site Characterization of High-Level Nuclear Waste Repositories* (excluding Section 2.1[b] and [c], and Section 17.1).

Four SNL QAPs were used to develop, document, and enter parameter information into the CCA PA Parameter Database: QAPs 9-1, 9-2, 9-4, and 9-5. QAP 9-2 contains the QA requirements for the selection and documentation of parameter values used in WIPP PA. Form 464, the WIPP Parameter Entry Form, is used in conjunction with QAP 9-2. Two QAPs are used to document the analysis and review of parameter values: QAP 9-1 and QAP 9-5. QAP 9-1 contains the QA requirements for conducting and documenting analyses, and QAP 9-5 contains QA requirements for conducting and documenting routine calculations. QAP 9-4 contains the QA requirements for the database management of parameter values used in WIPP PA.

### 3.1.4 Contractor QA Program

Work performed by SNL contractors must meet the same rigorous QA requirements as work performed by SNL. Through the SNL procurement process, upper-tier QA requirements are passed down to contractors. Contractors may develop their own QA program that meets the requirements of DOE/CAO QAPD, or they may work directly under the SNL QA procedures. Implementation of QA requirements by contractors is verified through the SNL audit and surveillance program.

## 3.2 Parameter Qualification

A parameter is considered processed (and thereby qualified) if it was developed under the qualified SNL QA program. A qualified parameter is defined as any parameter that is developed under an approved WIPP QA program and, if applicable, is traceable to qualified data.

### 3.2.1 QAP 9-2

As described in Section 4.2 (Tables 4 and 5), for Category 1 parameters, the parameter value is usually based on qualified empirical data. These parameters are entered into the PA Database and have the concurrence of the PI, the PAA, and the PTL; or they are justified, documented, and undergo technical and QA review per QAP 9-1, "Quality Assurance Requirements for Conducting Analyses."

For most Category 2 parameters, the parameter is traceable to the CAO Transuranic (TRU) Waste Baseline Inventory Report (BIR), also known as the TWBIR, which is consistent with the waste component limits described in Appendix WCL of the CCA.

For Category 3 parameters, the parameter value is based on information generally accepted by the scientific and engineering community. This information comes from handbooks and references appropriate to the field.

Category 4a parameters are model configuration parameters that are analogues to Category 1 parameters based on empirical data. For Category 4a parameters (analogs), the parameter value is entered into the PA Database and has the concurrence of the PI, PAA, and PTL; or it is justified, documented, and undergoes technical and QA review per QAP 9-1, "Quality Assurance Requirements for Conducting Analyses."

For Category 4b parameters (model configuration parameters), the parameter value is justified in, and technically reviewed as part of, the analysis documentation for the appropriate code per SNL QAP 9-1. Table 3 contains the names and WPO numbers for the analysis packages for codes used in the CCA calculations.

Table 3. CCA Code Analysis Packages and WPO Numbers

| CCA Code Analysis Package Title | WPO # |
|---|---|
| Analysis Package for the Salado Flow Calculations (Task 1) of the Performance Assessment Analysis Supporting the Compliance Certification Application | 40514 |
| Analysis Package for the Salado Transport Calculations (Task 2) of the Performance Assessment Analyses Supporting the Compliance Certification Application | 40515 |
| Analysis Package for the Culebra Flow and Transport Calculations (Task 3) of the Performance Assessment Calculations Supporting the Compliance Certification Application | 40516 |
| Analysis of the Generation of Transmissivity Fields for the Culebra Dolomite Compliance Certification Application | 40517 |
| Analysis Package for the BRAGFLO Direct Release Calculations (Task 4) of the Performance Assessment Calculations Supporting the Compliance Certification Application | 40520 |
| Analysis Package for the Cuttings and Spallings Calculations (Tasks 5 and 6) of the Performance Assessment Calculations Supporting the Compliance Certification Application | 40521 |
| Analysis Package for the CCDF Construction (Task 7) of the Performance Assessment Calculations Supporting the Compliance Certification Application | 40524 |

The code analysis packages contain the justification and rationale for the Category 4b parameters. Because the code analysis packages were not finalized until after the codes were run, there is no link from the Form 464 to the analysis packages for the 4b parameters. However, a memorandum was written to provide the traceability link (Martell to Howarth, March 3, 1997: "Cross Reference of Category 4B Parameters to the Analysis Package for the Code Utilizing the Parameter"). A copy of this memorandum is included as Appendix E and can be found in the correspondence files for the Form 464s in the SWCF. In addition, the traceability links from the Form 464s to the code analysis packages are contained in the EPA Parameter Database for the Category 4b parameters.

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# 4. Parameter Development Process

The CCA probabilistic codes frequently require input values that define a statistical distribution for each parameter. Developing parameter distributions begins with the assignment of an appropriate distribution type, which is dependent on the type, magnitude, and volume of data or information available. The development of the parameter distribution values may require interpretation or statistical analysis of raw data, combining raw data with literature values, scaling of laboratory or field data to fit code grid mesh sizes, or other transformations. Parameter development and documentation of the development process were very complicated, especially for those parameters based on empirical data; they required the integration of information from SNL code sponsors, PTLs, PAAs, and experimental PIs. This section contains a discussion of the parameter development process, roles and responsibilities, and lessons learned. Discussions of parameter documentation, traceability, and retrieveability are contained in Section 7.

As described in Appendix PAR of the CCA, the development of parameter values follows SNL WIPP QAP 9-2. The procedure includes documentation of parameter development by the individual responsible for completion of a particular experimental investigation, system design, or implementation of a performance assessment model.

Following QAP 9-2, any requests from PAAs for a new parameter or a modification to a parameter that existed in the 1992 PA calculations are sent to the PTL. After reviewing the request, the PTL elicits the PI or PAA for information to support the parameter. When a source for the parameter is identified, the information generated by the PI or PAA is processed by the PTL, who completes the information portion of Form 464 for the particular parameter. (Note that many of the fields described here for the CCA PA Parameter Database did not exist for the 1992 PA calculations.)

Form 464, the WIPP Parameter Entry Form, is the official documentation from the PTL to the Database Administrator (DBA) , which provides information to be entered into the PA CCA database for a particular parameter. Upon completion of the appropriate portions of Form 464, the PTL provides the form and any supporting information to the DBA. Form 464 and any attached supporting information comprise the PRP. Each PRP is assigned a WPO number and submitted to the SWCF.

## 4.1 Roles and Responsibilities

As described in QAPs 9-2 and 9-4, several individuals are responsible for the development, documentation, and data entry of parameters for the CCA. A description of the responsibilities is contained in the following subsections.

### 4.1.1 Database Administrator

The Database Administrator is the individual responsible for maintaining the software and security of data entered into the CCA PA Parameter Database: software security, availability, and accessibility. Database administration responsibilities also include ensuring that all parameter documentation from the PTL is placed in the SWCF, working closely with the PTL to ensure timely updates to the database to meet schedules, and working with the configuration management system (CMS) personnel to make the latest version of the database available to run the PA codes.

### 4.1.2 Data Cataloger

The Data Cataloger is the individual responsible for entering parameters and/or parameter information into the CCA PA Parameter Database.

### 4.1.3 Database Reviewer

The Database Reviewer is any person, other than the Data Cataloger or PTL, who inspects the inputs and/or updates made by the Data Cataloger.

### 4.1.4 Parameter Task Leader

The Parameter Task Leader works cooperatively with appropriate PIs and PAAs to develop needed parameter values and distributions. Development generally proceeds according to the process described in Section 4.2.2 (Figure 3). The PTL is also the individual within the SNL WIPP project who coordinates the development of parameters, has the responsibility for classifying parameters according to category, and approves requests for parameter entries into the controlled database. PTLs should have a broad technical understanding of the data and other available source information, conceptual models, and codes used in the project so that they understand the parameter in terms of the reasonableness of the parameter distribution values and the appropriateness of its use in the context of the model.

### 4.1.5 Principal Investigator

The Principal Investigator is the SNL WIPP staff member responsible for the completion of a particular scientific/experimental investigation or design.

### 4.1.6 Requester

The Requester is any individual within the WIPP project who requests a parameter entry, modification, or correction to the controlled database.

### 4.1.7 Performance Assessment Analyst

The Performance Assessment Analyst is the individual responsible for performing a numerical modeling exercise as part of the overall WIPP CCA PA. The PAA is sometimes referred to as the "Code Sponsor."

## 4.2 Parameter Development by Category

### 4.2.1 Background

When the development of CCA parameters began, many CCA codes were still being developed or had not completed the software lifecycle process, the list of parameters required for many codes was incomplete, and some supporting data were still being developed and/or analyzed. However, it was clear that parameter distributions and supporting documentation, including the rationale or justification for the particular parameter distribution chosen, would be required to meet the regulatory requirements for all CCA codes.

In October 1995, when the parameter development process first began, there were no QAPs in place to define or regulate the elaboration or documentation of parameter development.

However, as in the 1992 PA calculations, a well-defined process was used to acquire, control, and document the information input to the CCA PA Parameter Database while appropriate QAPs were finalized.

The development and documentation of parameter distribution information was dependent on the information known about the data values and their implementation in the codes of information sources available (e.g., empirical data, literature values, regulatory mandated values, general engineering knowledge, or combinations of source information). Note that, prior to the CCA, parameters used in WIPP PAs were not categorized. Categories 1, 2, 3, 4a, 4b, and 5 were initially conceptualized in August 1995; the definitions were formalized according to QAP 9-2 and the development of Form 464.

During the initial development and documentation of parameters, QAP 9-2, Revision 1 was in effect and contained the description of parameter categories as defined below in Table 4. Later in the parameter development and review process, the need to provide more definitive descriptions of the parameter categories was identified. The category descriptions were revised as documented in QAP 9-2, Revision 2, as shown in Table 5. The revised category descriptions did not lead to a change in the category of any parameters.

In an attempt to accelerate the parameter development and documentation process, and to meet the first CCA calculation schedule milestone (BRAGFLO calculations), teams of PIs, PAAs, managers, and others met to determine the information necessary for the BRAGFLO calculations (i.e., data and statistical distributions and other information supporting a choice of parameters). The group discussed the scope of information needed, the types of QA procedures that existed and those that would be needed, the format of the information, and the roles and responsibilities of individuals.

Table 4. Parameter Categories as Described in QAP 9-2, Revision 1

| Category | Description |
|---|---|
| 1* | Parameters that do not fall into Categories 2 through 5 but are necessary to WIPP PA calculations. |
| 2 | Parameters representing the inventory of the waste to be emplaced in the WIPP as defined in the WIPP *Transuranic Waste Baseline Inventory Report* (CAO-94-1005). |
| 3 | Parameters representing physical constants (e.g., the half-life of a radionuclide, gravitational constant). |
| 4a | Parameters that are assigned based on an assumed correlation of properties between similar materials. |
| 4b | Parameters that are model configuration parameters. |
| 5 | Parameters that are not used in current compliance calculations. |

*Note: The CCA PA Parameter Database contains a few parameters for which the category is listed as "1B." When parameters were initially categorized, the Category 1 parameters were subdivided. As the categorization process evolved, that subdivision was eliminated and the "1A" and "1B" parameters were reclassified as "1". Thus parameters categorized as a "1A" or "1B" are the same as Category 1 parameters.

Table 5. Parameter Categories as Described in QAP 9-2, Revision 2

| Category | Description |
|---|---|
| 1 | Parameters based on site-specific information used as initial input to a WIPP PA numerical model that specifies the physical, chemical, or hydrologic properties of the rock formations, seals, backfills, and waste form, or any other natural or engineered feature of the WIPP. |
| 2 | Parameters representing the inventory of the waste to be emplaced in the WIPP as defined in the WIPP *Transuranic Waste Baseline Inventory Report* (CAO-94-1005). |
| 3 | Parameters representing precisely known, tabulated physical constants (e.g., the half-life of a radionuclide, gravitational constant). |
| 4a | Parameters that are assigned based on a similarity of properties between similar materials or features. |
| 4b | Parameters that are model-configuration parameters not based on specific WIPP properties or features but are needed to make PA models run (e.g., time-step limits). |
| 5 | Parameters not used in current compliance calculations. |

Because of the large number of parameters, the teams subdivided the parameters into twelve groups based on the experimental programs that provided data, as shown in Table 6. Five groups of parameters would be needed by February 1, 1996 for BRAGFLO runs: (1) Salado Flow, (2) Non-Salado Flow, (3) Shaft Seals, (4) Gas Generation, and (5) Disposal Room. The remaining seven groups of parameters were needed for codes that were run after the BRAGFLO calculations: (6) Dissolved Actinide Retardation, (7) Colloidal Actinide Concentration, (8) Colloidal Actinide Retardation, (9) Dissolved Species, (10) Cuttings, (11) Non-Salado Culebra Transmissivity, and (12) Non-Salado Physical Transport.

Table 6. Parameter Development Groups

| Group Number | Parameter Group |
|---|---|
| 1 | Salado Flow |
| 2 | Non-Salado Flow |
| 3 | Shaft Seals |
| 4 | Gas Generation |
| 5 | Disposal Room |
| 6 | Dissolved Actinide Retardation |
| 7 | Colloid Actinide Concentration |
| 8 | Colloid Actinide Retardation |
| 9 | Dissolved Species |
| 10 | Cuttings |
| 11 | Non-Salado: Culebra Transmissivity Zone |
| 12 | Non-Salado: Physical Transport |

Without formal procedures in place to follow initially (QAPs 9-2 and 9-4 were not complete at the time the accelerated parameter development process began), the five groups supplying parameters for the initial BRAGFLO runs met individually in the autumn of 1995. The groups worked to identify required parameters, discuss available data, determine ownership for each parameter, and develop a parameter submittal process. The PAAs identified the parameters necessary to implement the codes. Once identified, the PAAs then teamed with the PTL and the appropriate PIs, who provided the status on data for specific parameters. The PIs identified new data or analyses that could be used to develop parameter distributions for the CCA calculations.

A PI or PAA, in conjunction with the PTL, was given ownership of each parameter and provided the necessary documentation for submitting the parameter distributions. In general, PIs were given joint ownership (with the PTLs) for the development of parameters derived from the data they collected and analyzed. The PIs were tasked with providing new data, mean or median values, and distributions for parameters under their ownership. Correspondingly, PAAs were given joint ownership (with the PTLs) for development of parameters necessary to run the codes (i.e., model configuration parameters), reference constant parameters whose values were taken directly from handbooks or technical literature, and parameters derived from interpretation of regulations or documents such as the WIPP BIR.

QAP 9-2, QAP 9-4, and Form 464 were developed during this time and were in place in late November 1995. QAP 9-2 formalized the parameter development and documentation process, and QAP 9-4 formalized the parameter entry process. Form 464 was used to document parameter information entry into the CCA PA Parameter Database.

Within the twelve parameter groups, the development and documentation of parameter values was dependent on the category assigned to the parameter. Details regarding parameter development and documentation for each parameter category are contained in the remainder of this section.

The development of parameter values followed QAP 9-2; the process is shown in Figure 3. The development of distribution values is discussed in Section 6.7.

### 4.2.2 Category 1—Parameters Based on Empirical Data

When data that support a particular parameter are identified, the PTL and the PAA meet with the appropriate PI, who then assembles a PI Parameter Package (PIPP). The PIPPs, which link the technical data records packages to Form 464, provide additional source information to support the parameter development documentation found in the PRP. The PIPPs are discussed in more detail in Section 6.10.1.

As shown in Figure 3, after the PI assembles a PIPP, it is provided to the PTL and a copy is submitted to the SWCF. The PTL then determines the appropriate parameter distribution from the information contained in the PIPP and completes Form 464. The PTL or designee then signs Form 464 and passes it to the PI and the PAA. If the PI and PAA concur with the distribution values selected, they also sign Form 464.

If more than one source of empirical data exist (e.g., anhydrite permeability data were available from two PIs; one providing laboratory data and the other providing field data to the PTL), each PI provides a PIPP to the PTL. Each PI also reviews the distribution developed by the PTL.

In some cases, a PI provided suggestions for parameter distribution to the PTL as part of the PIPP. The PTL reviewed the suggested distribution. If statistically appropriate, that distribution was entered on Form 464; if not, the PTL developed an alternative distribution using the available data or other information, as described in Section 6.7. The signature of the PI on Form 464 indicates concurrence with the distribution values selected by the PTL in such cases.

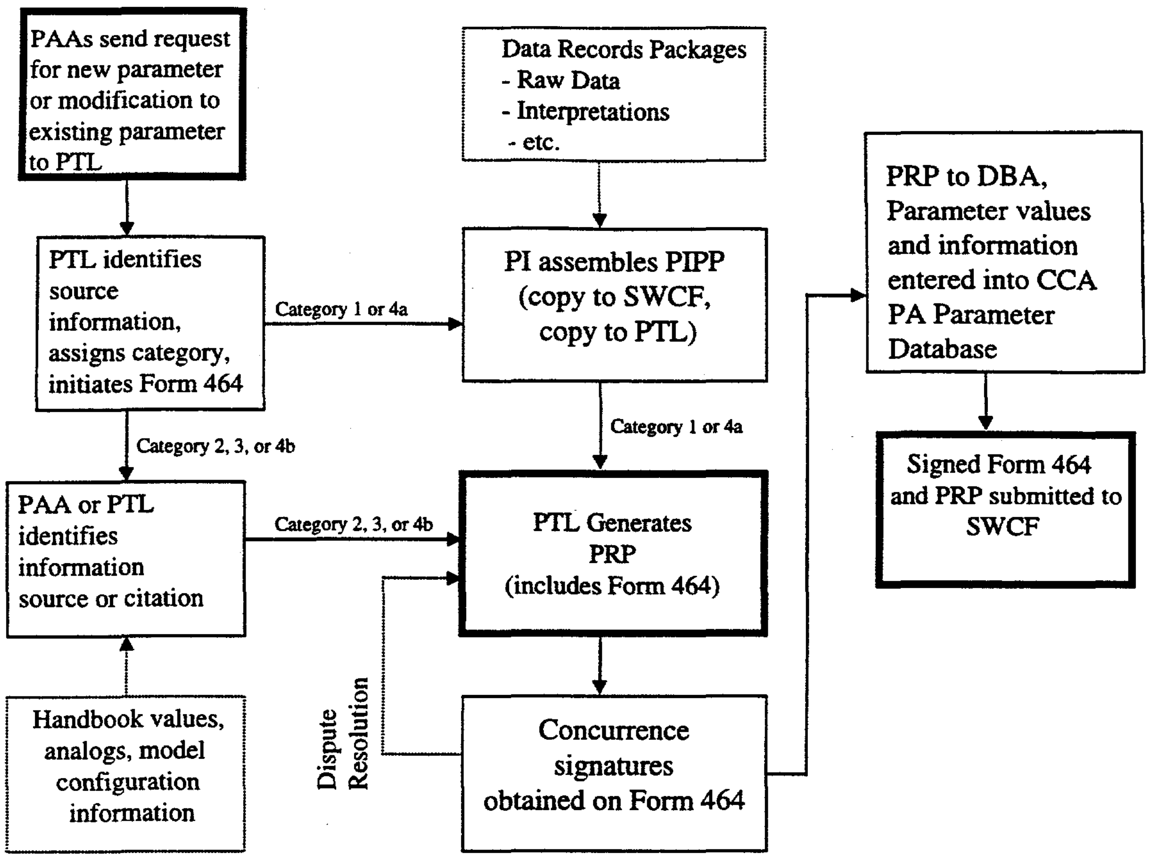


Figure 3. Parameter development process.

#### 4.2.2.1 Dispute Resolution

If the PI and PAA do not concur on the distribution values determined by the PTL, a dispute resolution meeting is convened and the PI, PAA, and PTL establish a mutually agreeable parameter distribution. Disputes regarding parameter distributions occurred in a very small number of cases (notably Marker Bed 139 Permeability and Porosity) but were easily resolved. Documentation of dispute resolution meetings and results are found in the PIPPs.

#### 4.2.2.2 Concurrence

For both Category 1 and Category 4a parameters, concurrence signatures are required for the PTL, PI, and PAA. When the PI assembles a PIPP, it is provided to the PTL. The PTL then determines the appropriate parameter distribution and completes Form 464. The PTL or designee then signs Form 464 and passes it to the PI and the PAA. If the PI and PAA concur with the distribution values selected, they also sign Form 464.

### 4.2.3 Category 2—Parameters Related to the Transuranic Waste Baseline Inventory

Each waste component shown in Table 7 is related to quantities reported in Revisions 2 and 3 of the TWBIR (DOE, 1995-1996) and is reflected in one or more parameters used in performance assessment calculations of Complementary Cumulative Distribution Functions (CCDFs). The relationship among waste components, waste characteristics, and performance assessment codes is illustrated in Figure 4.

Table 7. Table of Waste Components Used in Performance Assessment[1]

| Characteristic | Component | Material Name | | Parameter Name |
|---|---|---|---|---|
| radioactivity in curies of each isotope | radioactivity in curies of each isotope | AM241<br>CM245<br>NP237<br>CS137<br>TH229 | RA226<br>U238<br>PU238<br>PU239<br>SR90, etc.[2] | EPAREL<br>ATWEIGHT<br>INVCHD<br>INVRHD<br>WUF |
| TRU radioactivity at closure | TRU emitting radionuclides, $t_{1/2} > 20$ years | AM241<br>CM245<br>NP237<br>CS137<br>TH229 | RA226<br>U238<br>PU238<br>PU239<br>PU240, etc.[2] | HALFLIFE<br>ATWEIGHT<br>INVCHD<br>INVRHD<br>WUF |
| redox potential | ferrous metals | STEEL<br>REFCON | | STOIFX<br>ASDRUM<br>DRROOM |
| gas ($H_2$) generation | ferrous metals | STEEL<br>REFCON | | CORRMCO2<br>HUMCOR<br>ASDRUM<br>DRROOM |
| microbial substrate: $CH_4$ generation | cellulose | WAS_AREA | | GRATMICI<br>GRATMICH<br>VOLRHW<br>VOLCHW |
| microbial substrate: $CH_4$ generation | plastics, rubber | WAS_AREA | | PROBDEG<br>VOLRHW<br>VOLCHW |
| microbial nutrients: $CH_4$ generation | sulfates | SULFATE | | QINIT |
| microbial nutrients: $CH_4$ generation | nitrates | NITRATE | | QINIT |
| microbial nutrients, $CO_2$ generation | sulfates | SULFATE | | QINIT |
| heat generation | RH-TRU | WAS_AREA | | VOLRHW |
| solvent action | water in the waste | WAS_AREA | | SAT_RBRN |
| microbial nutrients, $CO_2$ generation | nitrates | NITRATE | | QINIT |
| electrochemical processes | Sulfates, nitrates phosphates, | SULFATE<br>NITRATE[3] | | QINIT |
| microbial substrate: $CO_2$ generation | cellulose | WAS_AREA | | GRATMICI<br>GRATMICH<br>VOLRHW<br>VOLCHW |
| microbial substrate: $CO_2$ generation | plastics, rubber | WAS_AREA | | PROBDEG<br>VOLRHW<br>VOLCHW |

[1] After Table WCA-2, Appendix WCA, Section WCA.2 of DOE, 1996.
[2] Examples are given of material names for isotopes and elements.
[3] Examples are given of material names for chemical compounds.

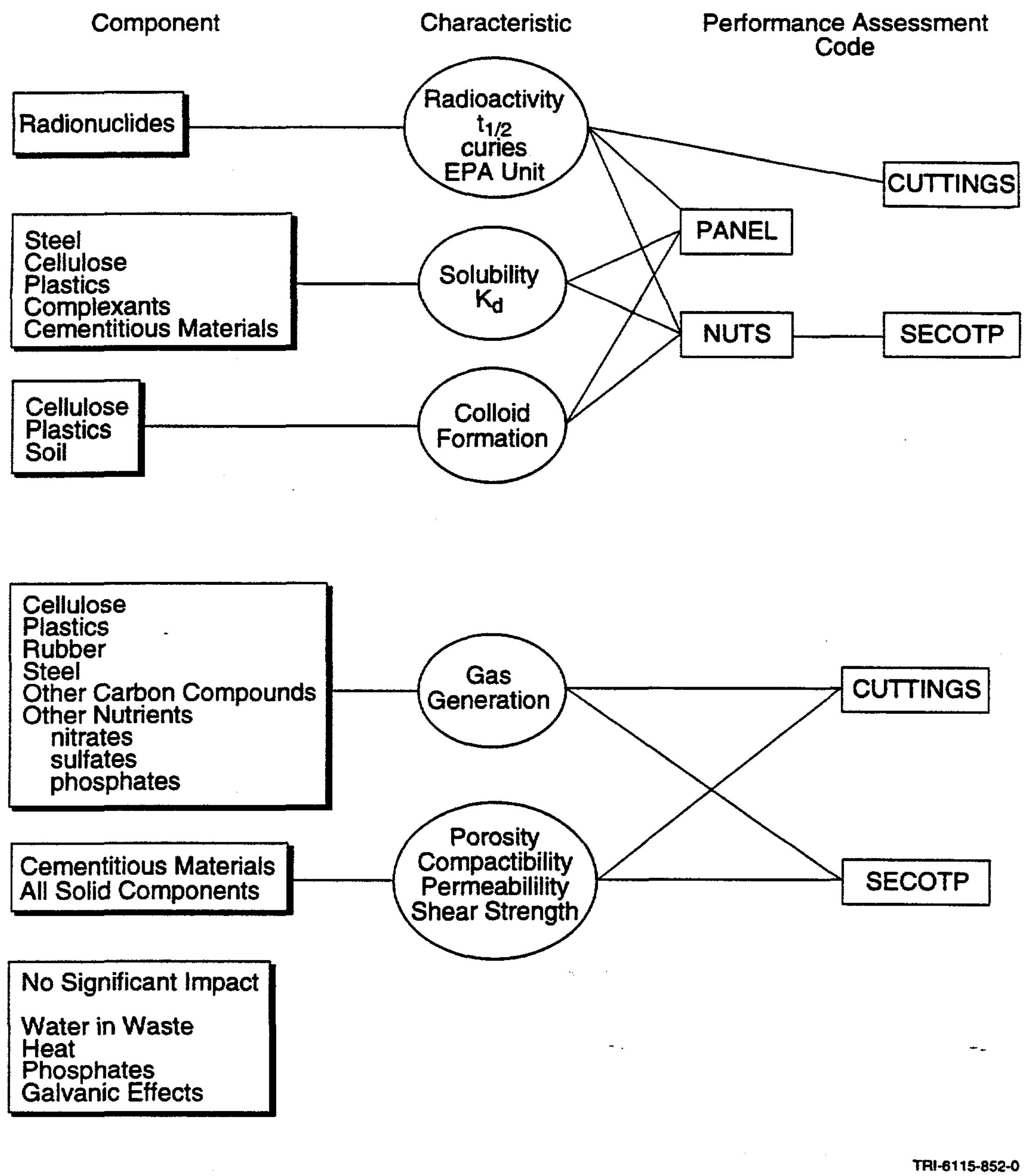


Figure 4. Components of the waste, examination characteristics, and performance assessment code using parameters for each characteristic (after Figure WCA-1, Appendix WCA, Section WCA.2 of DOE, 1996).

Explanations of parameter development and documentation for parameters involving the radionuclide inventory and parameters related to gas generation are found in Sections 6.10.1.2.2 and 6.10.1.2.3. Detailed explanations of the use of these parameters in performance assessment may be found in Appendices SOTERM (Section SOTERM.7) and WCA of the CCA and in the Analysis Packages for the codes CUTTINGS_S, PANEL, and NUTS.

### 4.2.4 Category 3—Literature, Handbooks, General Engineering/Scientific Knowledge

Parameters whose source information can be found in technical literature and scientific handbooks, or are based on general engineering or scientific knowledge, comprise the Category 3 subgroup. These parameters were constants and were usually specified by the PAAs. Concurrence is required of the PAA and PTL for Category 3 parameters.

For these parameters, the information from the source was entered in Form 464 and a citation reference was included on Form 464. A copy of the page from the source document was stapled to Form 464 to complete the PRP. If some type of minor calculation was required (e.g., unit conversion), the PRP also contained the calculation and the signature of the person who performed the technical review of the calculation per SNL QAP 9-5.

### 4.2.5 Category 4a—Analogues

Category 4a parameters are analogues, and supporting information may be linked back to Category 1 parameters or other supporting information. These parameters were jointly specified by the PAAs and PIs. Concurrence is required of the PI, PAA, and PTL for Category 4a parameters.

Documentation of the development of Category 4a parameters is contained in the PRP (see Section 7), referenced in the "Source" block of Form 464, or contained in the PA Code Analysis Packages. Because the PA Code Analysis Packages were not complete at the time the Form 464s were completed and used, there is no direct link to these analysis packages on Form 464. Listings of the PA Code Analysis Packages and the WPO number of each were given in Table 3.

### 4.2.6 Category 4b—Model Configuration

Category 4b parameters are primarily model configuration parameters. These parameters were the responsibility of the PAA. Concurrence on Form 464 is required of the PAA and PTL for all Category 4b parameters.

Documentation of the development of Category 4b parameters is contained in the PRP (see Section 7), referenced in the "Source" block of Form 464, or contained in the PA Code Analysis Packages. Because the PA Code Analysis Packages were not complete at the time the Form 464s were completed and used, there is no direct link to these analysis packages on Form 464. Listings of the PA Code Analysis Packages and the WPO number of each were provided in Table 3.

#### 4.2.6.1 4B Memo (Appendix E)

Because the PA Code Analysis Packages were not complete at the time the Form 464s were completed and used, there is no direct link to these analysis packages on Form 464.

Because the code analysis packages had not completed final review and publication at the time the CCA codes were run, according to QAP 9-2 they could not be referenced directly as a source on Form 464.

To provide a direct link from the PRP to the analysis packages, a memorandum was written documenting which parameters were addressed in which analysis packages; the memorandum was placed in the correspondence file (in the SWCF) for the PRPs and is included in Appendix E. A second link was provided by the inclusion of a reference to the WPO number of the analysis packages in the "Additional Sources" table of the EPA Parameter Database, which identifies Technical Traceability Documents (see Section 7 and Appendix M2).

### 4.2.7 Category 4b—Legacy and Placeholder

Two groups of parameters, both subsets of the Category 4b parameters, fell outside the bounds of QAP 9-2: legacy and placeholder parameters. Legacy parameters are those that had the same values or distributions as in the 1992 PA or other calculations run prior to the CCA calculations. Placeholder parameters are those that are required to run the code but have no effect on the calculation; they are essentially "spacers" in the parameter input records.

Because they were exempt from QAP 9-2 (QAP 9-2, covers "new" and "modified" parameters as they relate to the 1992 PA), parameter development and citations of source information for the legacy parameters are found in the 1992 PA documentation or in earlier documents. The QAP 9-2 and Form 464 process did not exist for parameters used in the 1992 PA.

Later, as a result of audits, surveillances, and reviews, it became apparent that the completion of a Form 464 for each parameter, including legacy and placeholder parameters, would be helpful for tracing parameter information in a manner consistent with the other parameters. The legacy and placeholder parameters were carefully reviewed by the appropriate PIs and PAAs: All were reclassified as Category 4b, and a Form 464 was filled out and filed in the SWCF for each. Although not specifically required by QAP 9-2, all parameters in the CCA PA Database now have an associated Form 464.

Documentation of the development of Category 4b parameters, including legacy and placeholder parameters, is contained in the PRP (see Section 7), referenced in the "Source" block of Form 464, or included in the PA Code Analysis Packages (see Section 4.2.7.1). Listings of the PA Code Analysis Packages and the WPO number of each were given is Table 3.

#### 4.2.7.1 "Legacy Memo" (Appendix F)

To provide a direct link from the PRP to the analysis packages, a memorandum was written documenting which parameters were addressed in which analysis packages; this memorandum was placed in the correspondence file (in the SWCF) for the PRPs and is included in Appendix E. In addition to the information related to all 4b parameters and contained in Appendix E, Appendix F contains three memoranda related to the legacy and placeholder parameters.

The first memorandum was from Tierney and Vaughn to File, dated June 17, 1996: "Designation of 'Legacy Parameters' and 'Placeholders' in the WIPP Parameter Database." This memorandum lists many legacy and placeholder parameters. During the parameter and CCA review, it was found to be incomplete and a second memorandum was required.

The second memorandum in Appendix F (Martell to Memo of Record, dated February 27, 1997: "Addenda to WPO#38568 SNL Internal Memo: M. Tierney and P. Vaughn to File, 6/17/96, Designation of 'Legacy Parameters' and 'Placeholders' in the WIPP Parameter Database") was written to clarify the information found in the first memorandum. It also provided a complete list of the legacy and placeholder parameters.

The third memorandum in Appendix F (Martell and Howarth to Memo of Record, dated September 2, 1997: "Addenda to 'Legacy Parameter' memorandum WPO#44202") was written to explain and document the rationale for placing legacy and placeholder parameters in the 4b category.

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# 5. CCA PA Parameter Database

The CCA PA Parameter Database contains most of the information that is recorded on a Form 464, including data values, associated models, all source information, category, and additional information documenting parameter information entry (such as data entry staff and entry date). The database does not include such information as the responsible PI, PAA, or PTL. The CCA PA Parameter Database uses a commercial (off-the-shelf) relational database application, Ingres SunOS Version 6.4/05. Note that there is no time stamp (date, time) for information input to the database except when values are changed or a parameter is deactivated. Strict control of read and write access and documentation trails ensures the security, integrity, and traceability of information into and out of the database.

## 5.1 Background

Prior to the development and implementation of the CCA PA Parameter Database, codes accessed information from a computational database (CDB) file that was produced from a secondary database, analogous to the CCA PA Parameter Database. In 1990 the GENPROP code was used to manually produce a CDB file. As the process evolved, parameters were collected into a centralized location called the secondary database (Rechard, 1992) and the codes began reading a CDB file (some parameters are still gained via input files or are hard-wired). The input file consisted of columns of data whose placement specification was defined by a header. A library of routines was created, enabling the codes to read the input file.

In 1991 Ingres was acquired and used to produce the CDB file and store the parameter information. The centralized location provided traceability and reproducibility of the parameters. The WIPP CCA PA Parameter Database was used for all code input parameters. The use of a common database for all CCA codes was intended to ensure consistency among the codes; that is, codes that utilized the same parameter (i.e., gravity, atomic weight) would use the same value. For the specific application of implementing conceptual models, the database tables were organized for high-volume calculational runs.

Thus the CCA PA Parameter Database, wipp_db, was created using Ingres. For the CCA calculations, the codes read data from a view produced by Ingres. It currently resides on the UNIX platform, Marvin. From Marvin, codes running on the Digital Equipment Corporation (DEC) Alpha Cluster can directly access pertinent information from the parameter database via an updated set of library routines.

The database contains information such as the parameter identification number (id), the name of the parameter material and property (idpram and idmtrl, respectively), units, distribution values, data source, and the activation status of the parameter. Other information found on Form 464, including the PI, PAA, or WID staff member responsible for the development of the parameter, is not stored in the database. The distribution values contained in the WIPP CCA PA Parameter Database were developed from interpreted data and other sources and, in essence, embody the disposal system conceptual models.

## 5.2 Structure of the CCA PA Parameter Database

The CCA PA Parameter Database was designed with a singular purpose: to provide the end user (the PA models) with necessary parameters. The CCA PA Parameter Database is (1) a relational database implemented in Ingres software, (2) a controlled database, and (3) an official WIPP project record.

Strict control of read and write access and audit trails ensures the security, integrity, and traceability of information used in the codes for CCA calculations. The CCA PA Parameter Database is a read-only database. Users are able to look at the information contained in the database, but they cannot make any changes.

### 5.2.1 Relational Database

In a relational database, related information can be stored in separate tables. Using the star-schema, key fields are then designed to define the relationship among the tables. In this manner, parameter information is not duplicated across multiple tables. The relationships may be one-to-one, one-to-many, or many-to-many. Note that the WIPP CCA did not utilize any many-to-many relationships.

As described in Section 2.2, a parameter is uniquely identified by a combination of its material name coupled with a property name, creating a material property name to describe a particular parameter. For the WIPP CCA the material is designated with an idmtrl alphanumeric and the property is designated by an idpram alphanumeric. For each unique set, the DBA assigned an id number, which establishes the relationship among the many tables.

The CCA PA Parameter Database contains all the information that is recorded on a Form 464 for a particular parameter, including distribution type, mean value, median value, standard deviation, minimum value, and maximum value, associated models, all source information, and category. It also contains information documenting data entry, such as the date the parameter changed and the name of the person authorized to make the change. For traceability, the WPO number for each parameter is stored, and for Category 1 and 4a parameters the WPO number of the primary PIPP is also included.

Figure 5 shows a typical one-to-one relationship that may exist within a parameter database. For each unique material identifier (idmtrl), defined in table **parameters**, a single entry will exist in the table **material**. This single entry consists of two fields: *idmtrl* and *material_description*, where *material_description* is an English translation of the *idmtrl*. The tables are related by the key field idmtrl.

Similarly, for each unique idpram, defined in table **parameters**, a single entry will exist in the table **property**. This single entry consists of three fields: *idpram*, *property_description* (where *property_description* is an English translation of the *idpram*), and *units*. The tables are related by the key field idpram. In this manner, each idmtrl and/or idpram is linked to its definition.

Figure 6 shows a typical one-to-many relationship that may exist within the parameter database. For each id, defined in table **parameters**, multiple entries may exist in table **sources** because a single parameter may have multiple sources. The tables are related by the key field id. Similarly, for table **values**, there may be multiple entries for certain distribution types, or no entries at all (e.g., constants).

The table **sources** may have a one-to-one (or one-to-many) relationship to other tables. In the example shown, one can determine the title and author of a parameter's information because a relationship exists between table **parameters**, table **sources**, and table **bibliography**. This can be compiled for either single or multiple parameters because the parameters are linked to table

**bibliography** through *id* and then the *refid*. Furthermore, one may find all parameters that have the bibliography listed as a reference.

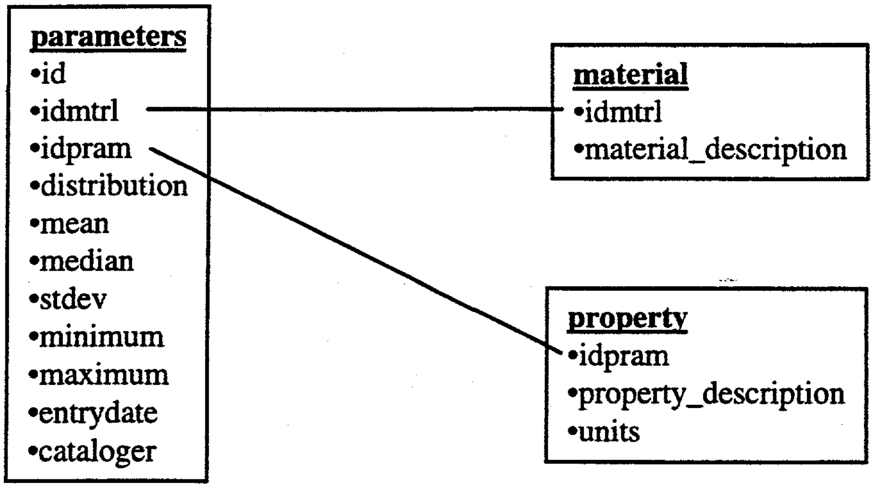


Figure 5. One-to-one relationship.

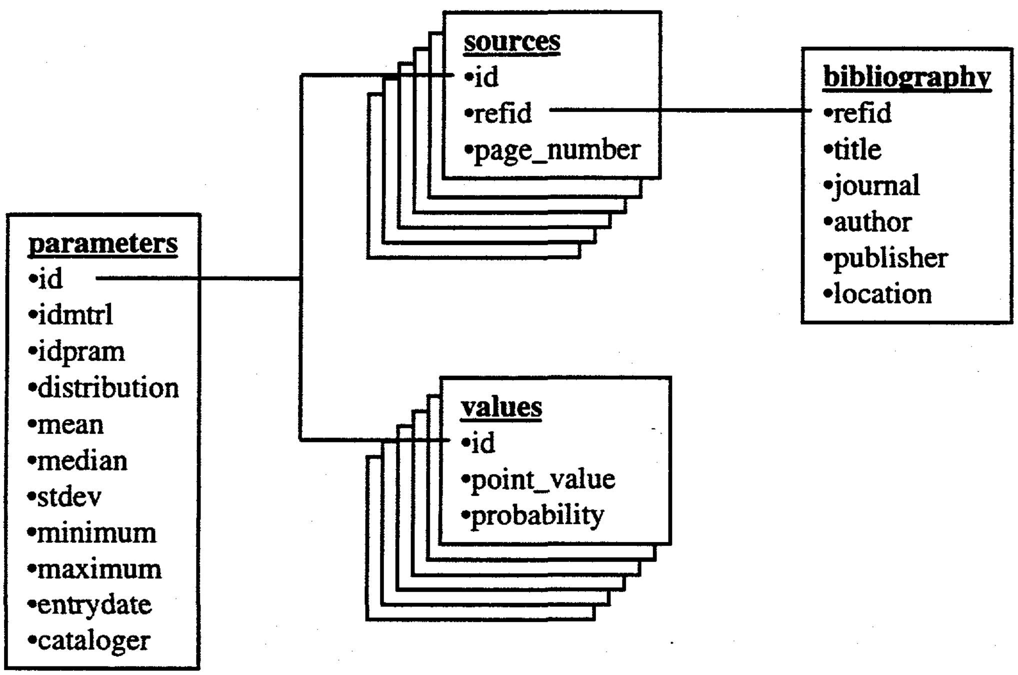


Figure 6. One-to-many relationship.

### 5.2.2 Views

Virtual tables, called views, were created in Ingres. These views, which are snapshots in time, are created from preexisting tables; they are *not* tables themselves. Related information from tables are joined together to form a view, as shown in Figure 7. In this example, information from Tables 1 through *n* are linked together to create a virtual table called *view*. The view does not have to consist of all of the information contained in all tables, but it contains preselected information. In the WIPP CCA the views were based on the CDB ASCII flat files, so the codes would be receiving the same type of information as previously received. Note that a view contains the most current information; if parameter information is updated in the underlying tables, it is reflected in the corresponding view.

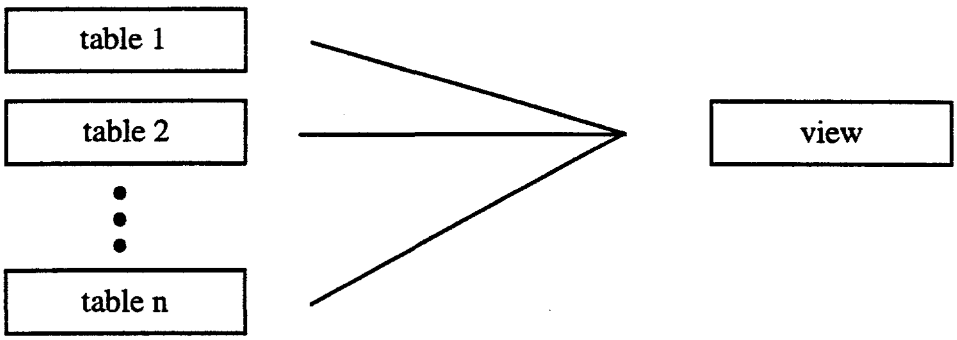


Figure 7. Diagram of a view.

### 5.2.3 Security

Strict control of read and write access and audit trails ensures the security, integrity, and traceability of information into and out of the database. Prior to the implementation of the Ingres database as the central CCA PA database, there was no control over the methods or persons updating the parameters. (Note that the DEC CMS provides traceability and reproducibility of the calculations, whereas the Ingres database provides an extra margin of security for the parameters.)

Although all code sponsors have some access to the VAX Alpha Cluster, not everyone has access to the UNIX machines. A generic userid "wipp" with password protection was created on the UNIX machine, Marvin. The password is maintained by the DBA and is not given to anyone else. Further, the "wipp" userid is defined without a home directory, so if someone tries to log on to Marvin, knowing both the userid and password, the message shown in Figure 8 is displayed and the user is disconnected. Ingres provides this additional security:

1. The DBA must define a valid user to Ingres. The user must already exist, via userid, within the UNIX environment. (Note: to gain access the WIPP PA Computational Support manager must approve a request to have access to the UNIX machines.)
2. The DBA must define the user to a particular database. Even if a user is defined to Ingres, the user can only access specified databases as set by the DBA. The authority to create tables is granted only to a limited number of personnel (currently only the DBA and DBA backup).
3. Finally, in order to access the information in an Ingres database table, the user must have been granted permission to a particular table or tables within a particular database. The default permission granted to valid users is read-only. Only personnel who enter data into the database are granted both delete and update permissions. When a table is frozen for a calculation (see Section 5.4.4), the delete and update permissions are replaced by read-only.

```
SunOS UNIX (marvin)
login: wipp
Password:
Last login: Fri Aug  8 13:52:47 from 132.175.137.133
SunOS Release 4.1.3_U1 (GENERIC) #2: Thu Jan 20 15:49:16 PST 1994
/bin/csh -f: No such file or directory
No shell
```

Figure 8. Logon attempt display.

## 5.3 Development of the CCA PA Parameter Database—Phased Approach

The CCA PA Parameter Database was developed using a phased approach. This approach for the CCA calculations allowed the loading of data for one code at a time. A schedule for the CCA calculations was used to prioritize the need to enter particular data, and the data required for a code were entered as they were received.

The phased approach was used because (1) some necessary parameters were not yet defined, (2) some codes had not completed the software qualification process, and (3) some experimental programs were not completed. A phased approach ensured parameter retrievability and traceability while allowing the flexibility to run different codes at different points in the process and to allow for changes to be made to a parameter after its original development.

Retrievability and traceability were maintained by freezing pertinent tables (see Section 5.4.4) needed by the code or codes, via views. If a code was reexecuted, the same set of parameter information would be available for retrieval. The views provided traceability because they were built from a discrete set of tables that were not altered after being frozen. Table 8 is a cross-reference for the CCA views and their requested purposes.

Table 8. Views Used in the CCA

| View Name | Requested Purpose |
|---|---|
| cca1 | Not Used |
| cca2 | BRAGFLO |
| cca3 | BRAGFLO for Disturbed Calculations |
| cca4 | BRAGFLO for Disturbed Calculations |
| cca5 | Source Term and Nuts for Disturbed Calculations |
| cca6 | BRAGFLO_DBR for Disturbed Calculations |
| cca7 | SECOTP2D for Disturbed Calculations |
| cca8 | CCDFGF for Disturbed Calculations |
| cca9 | PTL Requested |
| cca10 | Nuts and Panel for Disturbed Calculations<br>(using corrected inventory to year 2033) |
| cca11 | PTL Requested |

## 5.4. Parameter Entry Process and Form 464

Because of the phased approach, there are multiple Form 464s for some parameters. Figure 9 illustrates the course of a Form 464 through its lifecycle. As shown, when a PI or PAA requests a new parameter or an update to an existing parameter, the PTL generates a Form 464 to authorize an update of the database or to authorize an error correction.

After completion of the appropriate portions of Form 464, the PTL provides that form and any supporting in formation (i.e., PIPP) to the DBA. The DBA oversees any changes and/or additions to the tables in the User Database. The PTL sends written notification to the DBA when the tables are frozen. All PRPs are assigned a WPO number and a paper copy is submitted to the SWCF.

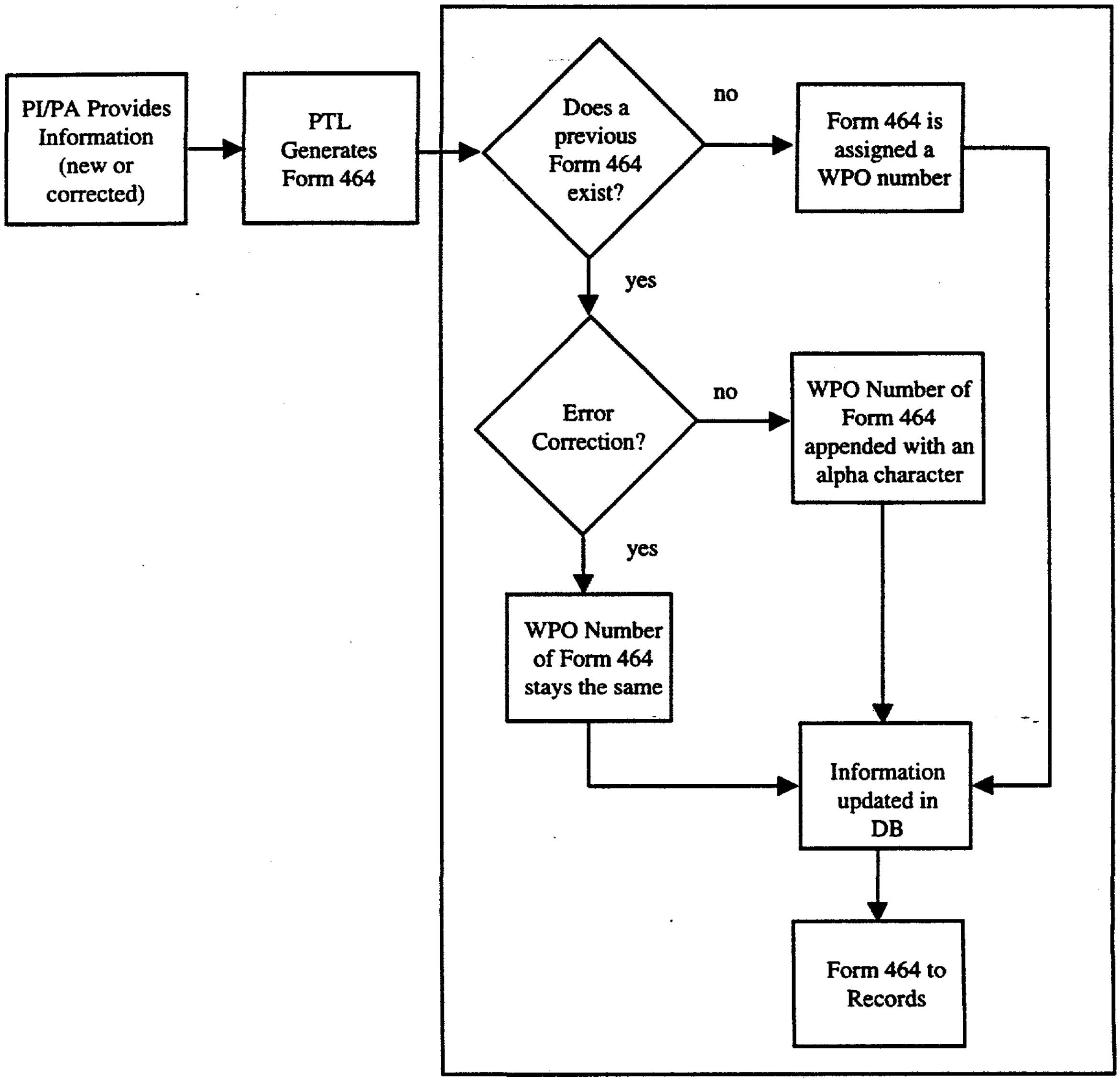


Figure 9. Form 464 generic lifecycle.

The DBA maintains two databases relevant to the CCA. The User Database contains the most recent parameter inputs to be used in the calculation. To ensure traceability of parameter values, version numbers are associated with tables in the database. Access to the database is restricted, as discussed previously in Section 5.2.3. The Master Database contains the most recent, finalized version of the parameter inputs, and only the DBA has write access to this database.

### 5.4.1 New Parameters

For a new parameter, the DBA makes a request to the SWCF for a WPO number unique to the new parameter. While awaiting the assignment of the WPO number by SWCF staff, the database entries are made. When the WPO number is received, it is entered into the database and handwritten on the Form 464 in the upper right corner. The Form 464 and any attachments are then placed in the SWCF as an official QA record.

### 5.4.2 Error Corrections

For an error correction, the WPO number of Form 464 is the same as the one denoted on the previous Form 464 because an error correction is not considered new or updated information. The PTL makes this correction using Form 464 or an internal memorandum, which is submitted to the SWCF and cross-referenced to the parameter in error.

### 5.4.3 Updated Parameters

A Form 464 is required for a name change or if the category or the numerical values (i.e., mean, median, standard deviation, lowrange, hirange, or distributed values) for a parameter are changed. In some cases a previous Form 464 existed that was correlated to a previously frozen set of tables (see Section 5.4.4). If the numerical value was updated, the following procedure was used to track multiple Form 464s for a single parameter.

The new Form 464 (for the update) was assigned the WPO number of the previous form with an alpha character suffix added to the WPO number on the upper right corner of Form 464. The updated form was processed and sent to the SWCF to be filed with previous Form 464s for that parameter.

For example, suppose the Form 464 for a new parameter is assigned WPO number 12345. This parameter will be used by a code later in the month. In the meantime, other codes were executed, using a frozen set of tables that included parameter 12345, although this parameter was not used by those codes. When a request is made to update the parameter value, the PTL creates a new Form 464 and sends it to the DBA for processing. The DBA verifies that the parameter already exists, adds the preassigned WPO number 12345 to Form 464, and adds the alpha character "A" to the end so that the new Form 464 has WPO 12345A in the upper right corner. The WPO number will remain the same, 12345A, until another update is required. If another update is required, the next Form 464 will be 12345B, and so on.

According to QAP 9-2, a Form 464 was not required for the legacy and placeholder parameters. However, auditors and technical and QA reviewers requested that, for consistency, a Form 464 be created for all parameters in the CCA PA Parameter Database. In response to their request, a Form 464 was created for each of the legacy and placeholder parameters. Note that a check-off box did not exist on Form 464 to denote this reason for creating a Form 464; the PTL thus checked the "major modification" box because it was the best choice available.

### 5.4.4 Freezing Database Tables

When a code calculation is scheduled to begin and all the parameters have been entered, the PTL issues a memorandum requesting that a specific database table be frozen. A view, a snapshot in time, is made of necessary parameter information and maintained. The process used to freeze a database table is described below (note that the database is not frozen; only the view that joins the tables specified by the PTL is frozen).

1. The PTL requests that certain tables be made unavailable for update.
2. All update and delete authority is removed from the specified tables; that is, only the DBA can change frozen tables, and this is strictly forbidden. The only access other than the DBA access is read-only.
3. A database view is created from the tables specified by the PTL. The wipp userid is given read-only access to the view.
4. A flat file is created from the view's structure. An electronic copy of the flat file is placed into the CMS and a paper hard copy is submitted to the SWCF as part of a disaster recovery initiative.
5. New tables are created from the previously frozen tables so that work may continue in updating parameters for other codes to utilize.

This process continues until the PTL issues a memorandum stating that the database itself is to be closed.

### 5.4.5 CCA Table Structures

The CCA PA Parameter Database is composed of several tables, shown in Table 9. Only two tables contained parameter information used by the codes.

### 5.4.6 Disaster Recovery

The Ingres databases are backed up every night to prevent data loss. If Ingres fails, any information lost is less than 24 hours old, so only a day's work would have to be recreated. If Marvin fails, a separate UNIX machine has been designated to mirror Marvin.

Table 9. Tables Utilized in the CCA

| Table Name | Table Description and Contents |
|---|---|
| parameters_xxxx | Contains a full description of the property denoted by the idpram.<br>▪ id - Used to join the parameter to its property description.<br>▪ pram_desc - A description of the property. |
| model_xxxx | Contains the name of the code/model for which the parameter is required.<br>▪ id - Used to join the parameter to the name of the code(s) it is utilized by.<br>▪ codename - The name of the code(s) for which the parameter is required. |
| docu_xxxx | Contains a reference id which relates a parameter to its source.<br>▪ id - Used to join the parameter to its reference(s) or source(s).<br>▪ refid - A 30-character representation of a unique source.<br>▪ pagenum - The page number of the citation. |

Table 9. Tables Utilized in the CCA

| Table Name | Table Description and Contents |
|---|---|
| biblio_xxxx | Contains a full citation of the source from which the parameter is based.<br>■ refid - Used to join the reference representation to its full citation.<br>■ title - The citation's title.<br>■ journal - If required, the name of the journal where the citation is found.<br>■ author - The author(s) of the citation.<br>■ editor - If available, the editor(s) of the citation.<br>■ date - The date the citation was published.<br>■ publisher - The publisher of the citation.<br>■ location - The location where the citation was published. |
| desc_xxxx | Contains the parameter information normally associated with a majority of the parameters.<br>■ id - A unique identifier assigned to a unique combination of material and property which define a parameter.<br>■ idmtrl - An 8-character (maximum) representation of a material.<br>■ idpram - An 8-character (maximum) representation of a property.<br>■ units - The units associated with the parameter.<br>■ distyp - The distribution type associated with a parameter.<br>■ mean - The mean value of the parameter.<br>■ median - The median value of the parameter.<br>■ stdev - The standard value of the parameter.<br>■ lowrange - The low range of the parameter.<br>■ hirange - The high range of the parameter.<br>■ active - A flag denoting whether or not the parameter is active.<br>■ impt - The category assigned to the parameter.<br>■ cataloger - The person who entered/updated/deactivated the parameter.<br>■ entrydate - The date the parameter's values were entered or updated or the date the parameter was deactivated.<br>■ class - Not used.<br>■ source - Not required. It was a shorthand way of determining who requested the parameter (PIxx or PAxx).<br>■ qualified - No longer used due to an Interim Change Notice (ICN) in QAPs 9-2 and 9-4. |
| values_xxxx | Contains the values of distributed values which cannot be accurately described via a maximum and minimum only.<br>■ id - Used to join the parameter to its distributed values.<br>■ pramval - The values to which a parameter can be distributed over when it cannot be accurately described by its low range and high range alone.<br>■ probability - The probability assigned to a distributed value.<br>■ idx - A numbering of the distributed values. |
| wpo | Contains the WPO number assigned to the parameter.<br>■ id - Used to join the parameter to its WPO number.<br>■ wpo_number - The number assigned to a parameter by the SWCF |
| materials_xxxx | Contains a full description of the material denoted by the idmtrl.<br>■ id - Used to join the parameter to its material description.<br>■ mtrl_desc - A description of the material. |

**In the left column, xxxx denotes the different versions of the table.**

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# 6. Form 464

Form 464 is issued by the PTL as the official WIPP Parameter Entry Form. Although it can be used as the starting point for tracing from the CCA PA Parameter Database to the supporting or source information for a parameter (see Section 7), its original intent was simply as a data entry form. Within Form 464 are numerous fields that are completed by the PTL, as well as numerous signature lines that signify concurrence, identify the data entry person, or show that the data was entered correctly. (Note that early versions of Form 464 are also referred to as WIPP Data Entry Forms.)

In some cases, a single parameter may have more than one Form 464, as discussed in Section 5.4.3. Parameters were developed in phases, and changes may have been made to a parameter after its original development. Thus a new Form 464 might have been generated to contain additional or superseding information. Only information contained on Form 464 is entered into the CCA PA Parameter Database. For illustration, a copy of a blank Form 464 is shown as Figure 10; each field of Form 464 is described in detail in the following sections.

## 6.1 Id

The id number is a sequential number assigned to a parameter by the DBA. Once an id number is assigned, even if the parameter is later deactivated because it was not used in the PA calculation, it is not used for another parameter.

## 6.2 Idmtrl, Idpram

A maximum of an eight-character alphanumeric identifies the material and property, respectively. Created and assigned by the PTL, the combination of idmtrl and idpram uniquely identify a parameter.

## 6.3 Descriptions of the Idmtrl and Idpram

Descriptions are statements describing the material or property represented. This field is limited to 30 characters in the CCA database.

## 6.4 Units

Units are the dimensions of the parameter as defined by the represented values.

## 6.5 Model

This field includes a list of the numerical models or software codes that use the parameter.

## 6.6 Category

The category alphanumeric assigned to each parameter classifies the parameter according to the general source of its supporting information, as shown in Table 5. A "1" was assigned to parameters based in some part on WIPP site-specific data, a "2" to parameters based primarily on the WIPP BIR, a "3" to parameters based on literature or handbook values, a "4a" to analog parameters, a "4b" to model configuration parameters, and finally a "5" to parameters that were used in the 1992 PA but would be deactivated and thus not used in the CCA runs.

| WASTE ISOLATION PILOT PLANT<br>Sandia National Laboratories | **WIPP Parameter Entry Form**<br>**Form Number: 464** **Effective: 09/12/96** |
|---|---|
| | Procedure: 9-2 Revision: 2 Page 1 of 1 |

☐ Major Modification ☐ Error Correction ☐ New ☐ Deactivation

Parameter: ______ Id: ______

Material: ______ Idmtrl: ______

Model: ______ Idpram: ______

Category: ______ Units: ______

Distribution:

Type: Mean: ______

Median: ______

Std Dev: ______

Values: Attachment: ☐ Yes ☐ No

Source:

Interpretation:

Qualified Parameter: ☐ Yes ☐ No ☐ Yes ☐ No

Parameter Entry Approved by:

| | | |
|---|---|---|
| Parameter Task Leader *(Print)* | *Signature* | Date |

Requester:

| | | |
|---|---|---|
| Requester *(Print)* | *Signature* | Date |

Concurrence: (Required for Category 1 and 4a Parameters Only)

| | | |
|---|---|---|
| Principal Investigator *(Print)* | *Signature* | Date |
| Performance Assessment Analyst *(Print)* | *Signature* | Date |

Entered by:

| | | |
|---|---|---|
| Entered By *(Print)* | *Signature* | Date |

Entry Checked by:

| | | |
|---|---|---|
| Entry Checked By *(Print)* | *Signature* | Date |

SWCF File Code: ______
WBS#

Figure 10. Copy of blank Form 464.

Two group of parameters fell outside the bounds of QAP 9-2: legacy and placeholder parameters. Legacy parameters are those that had the same values or distributions as in the 1992 PA or other calculations run prior to the CCA. Placeholder parameters are those that are required to run the code but have no effect on the calculation. Because they were exempt from QAP 9-2 (which covers "new" and "modified" parameters as they relate to the 1992 PA), parameter development and citations of source information were found in the 1992 PA documentation or in earlier documents. The QAP 9-2 and Form 464 process did not exist prior to the CCA (1996).

Later, as a result of audits, surveillances, and technical reviews, it became apparent that the completion of a Form 464 for each parameter, including legacy and placeholder parameters, would be helpful for tracing parameter information in a manner consistent with the other parameters. The legacy and placeholder parameters were carefully reviewed by the appropriate PIs and PAAs. All were reclassified from Category 4 to Category 4b, and a Form 464 was completed for each and filed in the SWCF. Although not specifically required by QAP 9-2, all parameters in the CCA PA Parameter Database now have an associated Form 464.

## 6.7 Distribution

This field contains the statistical distribution assigned to a particular parameter (e.g., Student's *t*, uniform, and lognormal). Parameter distributions are assigned by the PTL as described in QAP-9-2. The process illustrated in Figure 11 was followed in the assignment of parameter distributions for the CCA PA Parameter Database. Four memoranda written by the PTL, which address distributions, are included in Appendix G of this report. The first memorandum (Martin Tierney to Distribution, dated March 21, 1996: "Distributions") discusses the various types of distributions assigned to parameters: cumulative, logcumulative, delta, normal, triangular, uniform, lognormal, and loguniform distributions. The second memorandum (Mary-Alena Martell to Distribution, dated April 4, 1996: "Student-T Distribution") discusses only the Student's *t* distribution. Each of the first two memoranda outlines the appropriate use for each distribution and includes a list of appropriate references.

The third memorandum (Martin S. Tierney to Distribution, dated April 16, 1996: "Development of Parameter Values Distribution Functions") includes a flow diagram that illustrates the parameter distribution development process.

The fourth memorandum in Appendix G (Martin Tierney and Mary-Alena Martell to Distribution, dated December 13, 1996: "On criteria for specifying CONSTANTs in the WIPP PA Parameter Database") contains reasons for choosing constant values for certain parameters and provides an informal discussion of those reasons.

In some cases, when providing data or other parameter information to the PTL, the PI may have suggested that a specific distribution be used for a parameter. The PTL reviewed the suggested distribution and determined which distribution type would be most appropriate. The PI's signature on Form 464 shows concurrence with the distribution type selected for the particular parameter by the PTL, even if it contradicts the distribution type originally suggested by the PI.

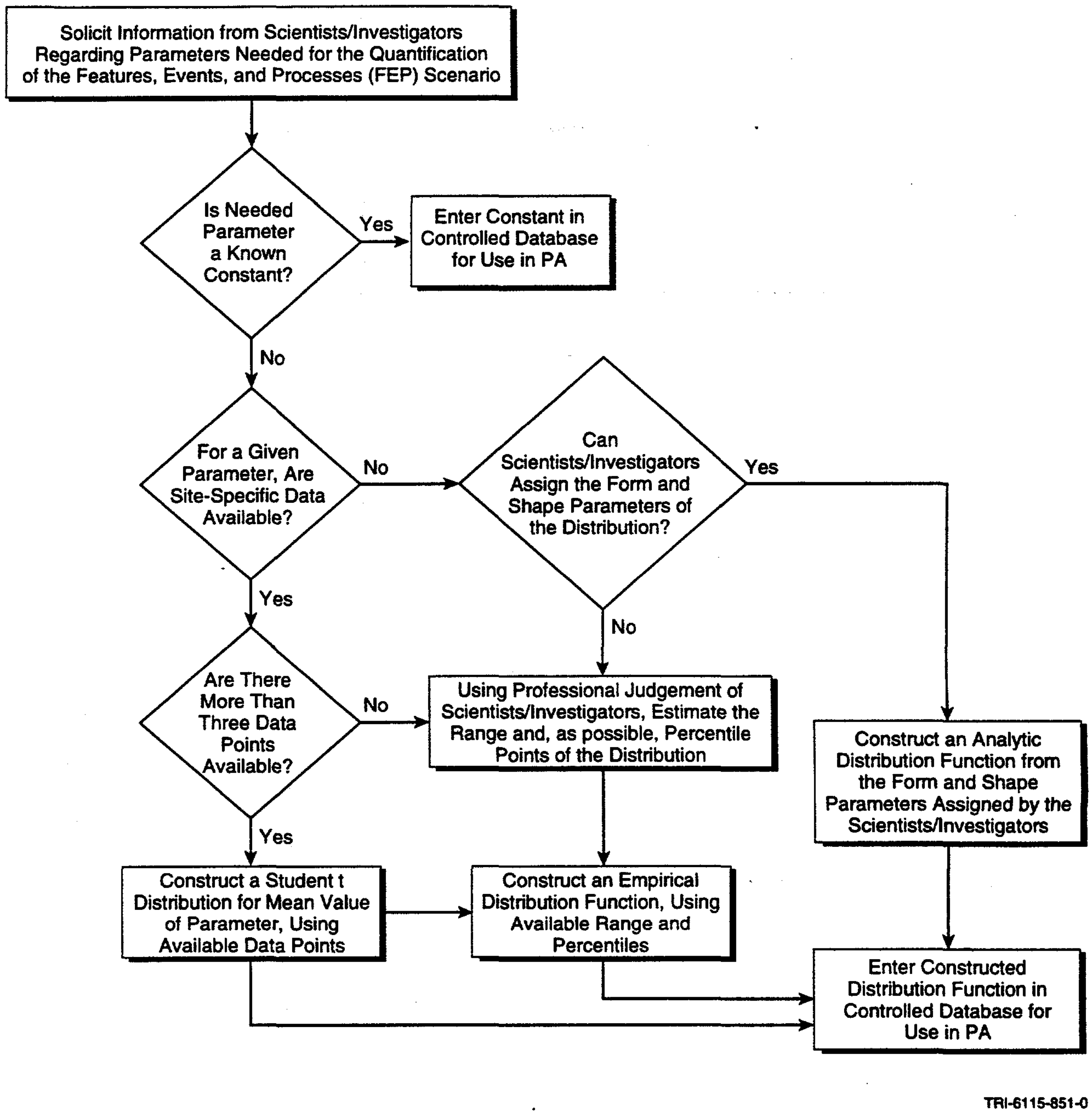


Figure 11. Parameter distribution flow diagram.

## 6.8 Type

This field contains the distribution type as determined by the PTL. Appendix G includes memoranda that contain detailed information regarding the types of distributions assigned to parameters for the CCA calculations.

## 6.9 Values

This field contains the numbers that define the parameter distribution and probability (e.g., mean, median, standard deviation, lowrange, hirange).

## 6.10 Source

This field contains information regarding the origin of the evidence or arguments supporting the parameter used. The source identified on Form 464 is the reference to documentation or data that support the parameter values *available to the PTL at the time the parameter was created or modified.* Source documentation may include memoranda, worksheets, technical data packages, PIPPs, literature, technical publications, handbooks, etc. The source document may be referenced with a citation or by a WPO number.

Category 1 parameters are typically supported by PIPPs and Technical Data Records Packages containing laboratory, field, and/or technical literature data. Category 2 parameters are primarily supported by information found in the WIPP BIR, and Category 3 parameters are supported by technical literature, handbooks, and textbooks. Category 4a parameters are analogues, and supporting information may be linked back to Category 1 parameters or other supporting information. Supporting information for Category 4b parameters, model configuration parameters, is found in the PA Analysis Packages. (The PRP correspondence file for 4b parameters contains a memorandum referencing the WPO number for the appropriate code analysis package).

### 6.10.1 Category 1

For most Category 1 parameters, the PIPPs are an important link in the traceability from Form 464 to the supporting Technical Data Records Packages that contain raw data, analyses, and other information. Because of the complexity of the development of some parameters, a format was suggested to PIs to assist in the organization and content of the PIPPs. Most PIPPs followed the prescribed format; however, this format was not used for all packages. The PIPPs for seals, gas generation, partition coefficient ($K_d$), blowout, and cuttings parameters include the same information as prescribed in the format guide, but they were organized differently for the sake of efficiency.

#### 6.10.1.1 Table of Packages

Table 10 lists all the PIPPs that support the CCA calculations. In some cases a single PIPP supports a single parameter; in other cases a PIPP may support multiple parameters (e.g., the seals PIPP); in still other cases a single parameter is supported by multiple PIPPs (e.g., the Salado anhydrite permeability parameters were developed from laboratory, and field data and separate PIPPs were assembled for the two sets of data). The "Source" field of Form 464 contains the link (the WPO number of the appropriate PIPP).

Table 10. Listing of PI Parameter Packages

| # | WPO# | PI/SOURCE OF PRP | GROUP | TITLE OF PARAMETER RECORD PACKAGE (PRP) | FILE CODE OF PRP IN AIMS DATABASE-PDD, WBS#, PKG IDENTIFIER | STATUS | W/DATA | DUAL STORAGE | AIMS TABLE OF CONTENTS |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 30598 | CHRISTIAN-FREAR, T. | SALADO | SALADO HALITE ROCK COMPRESSIBILITY FROM ROOM Q ANALYSIS | PDD, 1.207.1, SALADO PKG#5 | C | YES | SWCF-A/SAIC | |
| 2 | 30599 | HOWARTH, S. | SALADO | SALADO ANHYDRITE GRAIN DENSITY | PDD, 1.2.07.1, SALADO PKG#15 | IP | YES | SWCF-A/SAIC | X |
| 3 | 30600 | HOWARTH, S. | SALADO | SALADO ANHYDRITE EFFECTIVE POROSITY | PDD, 1.2.07.1, SALADO PKG#11 | IP | YES | SWCF-A/SAIC | X |
| 4 | 30601 | HOWARTH, S. | SALADO | SALADO HALITE POROSITY | PDD, 1.2.07.1, SALADO PKG#8 | IP | YES | SWCF-A/SAIC | |
| 5 | 30603 | HOWARTH, S. | SALADO | SALADO ANHYDRITE PERMEABILITY IN THE X-DIRECTION | PDD, 1.2.07.1, SALADO PKG#13 X-DIR | IP | YES | SWCF-A/SAIC | X |
| 6 | 30605 | HOWARTH, S. | SALADO | SALADO ANHYDRITE PERMEABILITY IN THE Y-DIRECTION | PDD, 1.2.07.1, SALADO PKG#13 Y-DIR | IP | YES | SWCF-A/SAIC | X |
| 7 | 30606 | HOWARTH, S. | SALADO | SALADO ANHYDRITE PERMEABILITY IN THE Z-DIRECTION | PDD, 1.2.07.1, SALADO PKG#13 Z-DIR | IP | YES | SWCF-A/SAIC | X |
| 8 | 30607 | DOTSON, L. | NON-SALADO | PERMEABILITY | PDD, 1.2.07.1, NON-SALADO PKG#21 | IP | YES | SWCF-A/SAIC | X |
| 9 | 30608 | DOTSON, L. | NON-SALADO | EFFECTIVE POROSITY | PDD, 1.2.07.1, NON-SALADO PKG#22 | IP | YES | SWCF-A/SAIC | X |
| 10 | 30611 | DOTSON, L. | NON-SALADO | BULK COMPRESSIBILITY | PDD, 1.2.07.1, NON-SALADO PKG#23 | IP | YES | SWCF-A/SAIC | X |
| 11 | 30640 | HURTADO, L.D. | MISC. | SHAFT SEALS PARAMETERS | PDD, 1.1.03.2.2, SHAFT SEALS BRAGFLO | IP | YES | SWCF-A/SAIC | |
| 12 | 30641 | CHRISTIAN-FREAR, T. | SALADO | VISCOSITY OF HYDROGEN GAS | PDD, 1.2.07.1, H2 VISCOSITY PKG#2 | C | YES | SWCF-A/SAIC | X |
| 13 | 30642 | CHRISTIAN-FREAR, T. | SALADO | KLINKENBERG CORRECTION FACTOR | PDD, 1.2.07.1, ANH H2 GAS PARAMETERS PKG#2 | C | YES | SWCF-A/SAIC | X |
| 14 | 30643 | CHRISTIAN-FREAR, T. | SALADO | ANHYDRITE TWO-PHASE PARAMETERS | PDD, 1.2.07.1, ANH 2-PHASE PARAMETERS PKG#10 | C | YES | SWCF-A/SAIC | X |
| 15 | 30713 | DOTSON, L. | NON-SALADO | PRESSURE | PDD, 1.2.07.1, PKG#24 NON-SALADO PRESSURE | IP | YES | SWCF-A/SAIC | X |
| 16 | 30721 | CHRISTIAN-FREAR, T. | SALADO | SALADO HALITE PERMEABILITY FROM ROOM Q ANALYSIS | PDD, 1.2.07.1, SALADO HALITE PERMEABILITY PKG#7 | C | YES | SWCF-A/SAIC | X |
| 17 | 30803 | CHRISTIAN-FREAR, T. | SALADO | SALADO DRZ INITIAL PRESSURE FROM ROOM Q ANALYSIS | PDD, 1.207.1, DRZ AND TRANSITION PRESSURE | C | YES | SWCF-A/SAIC | X |
| 18 | 30819 | WANG, Y. | MISC. | GAS GENERATION PARAMETERS REQUIRED FOR BRAGFLO | PDD, 1.1.09.1.1, ESTIMATES OF GAS GENERATION | IP | YES | SWCF-A/SAIC | |
| 19 | 31070 | FREEZE, G. | NON-SALADO | CASTILE BRINE RESERVOIR PERMEABILITY | PDD, 1.2.07.1, PKG#19-A, CASTILE BRINE, PERMEABILITY | IP | YES | SWCF-A/SAIC | X |
| 20 | 31072 | FREEZE, G. | NON-SALADO | CASTILE BRINE RESERVOIR PRESSURE | PDD, 1.2.07.1, PKG#19-B, CASTILE BRINE, PRESSURE | IP | YES | SWCF-A/SAIC | X |
| 21 | 31082 | FREEZE, G. | NON-SALADO | CASTILE BRINE RESERVOIR VOLUME | PDD, 1.2.07.1, PKG#19-C, CASTILE BRINE, VOLUME | IP | YES | SWCF-A/SAIC | X |
| 22 | 31083 | FREEZE, G. | NON-SALADO | CASTILE BRINE RESERVOIR POROSITY | PDD, 1.2.07.1, PKG#19-D, CASTILE BRINE, POROSITY | IP | YES | SWCF-A/SAIC | X |
| 23 | 31084 | FREEZE, G. | NON-SALADO | CASTILE BRINE RESERVOIR ROCK COMPRESSIBILITY | PDD, 1.2.07.1, PKG#19-E, CASTILE BRINE, COMP. | IP | YES | SWCF-A/SAIC | X |
| 24 | 31167 | ECONOMY, K. | NON-SALADO | CULEBRA PERMEABILITY | PDD, 1.2.07.1, NON-SALADO, PKG#21, CULEBRA PERM. | IP | YES | SWCF-A/SAIC | X |
| 25 | 31168 | ROBERTS, R. | SALADO | BRINE VISCOSITY | PDD, 1.2.07.1, SALADO, PKG#1, BRINE VISCOSITY | IP | YES | SWCF-A/SAIC | X |
| 26 | 31171 | DOMSKI, P.S. | SALADO | BRINE WTF | PDD, 1.2.07.1, SALADO, PKG#1, BRINE WTF | IP | YES | SWCF-A/SAIC | X |
| 27 | 31174 | ROBERTS, R. | SALADO | BRINE COMPRESSIBILITY | PDD, 1.2.07.1, SALADO, PKG#1, BRINE COMPRESSIBILITY | IP | YES | SWCF-A/SAIC | X |
| 28 | 31175 | ROBERTS, R. | SALADO | BRINE DENSITY | PDD, 1.2.07.1, SALADO PKG#1, BRINE DENSITY | IP | YES | SWCF-A/SAIC | X |

Table 10. Listing of PI Parameter Packages (continued)

| # | WPO# | PI/SOURCE OF PRP | GROUP | TITLE OF PARAMETER RECORD PACKAGE (PRP) | FILE CODE OF PRP IN AIMS DATABASE- PDD, WBS#, PKG IDENTIFIER | STATUS | W/DATA | DUAL STORAGE | AIMS TABLE OF CONTENTS |
|---|---|---|---|---|---|---|---|---|---|
| 29 | 31181 | CHRISTIAN-FREAR, T. | SALADO | DRZ INITIAL BRINE SATURATION FROM ROOM Q ANALYSIS | PDD, 1.2.07.1, SALADO, PKG#16, DRZ BRINE RM Q | C | YES | SWCF-A/SAIC | |
| 30 | 31184 | CHRISTIAN-FREAR, T. | SALADO | DRZ POROSITY FROM ROOM Q ANALYSIS | PDD, 1.2.07.1, SALADO, PKG#16, DRZ POROSITY | C | YES | SWCF-A/SAIC | X |
| 31 | 31185 | DOMSKI, P.S. | SALADO | ANHYDRITE PRESSURE | PDD, 1.2.07.1, SALADO, PKG#12, ANHYD PRESSURE | IP | YES | SWCF-A/SAIC | X |
| 32 | 31186 | DOMSKI, P.S. | SALADO | ROCK COMPRESSIBILITY | PDD, 1.2.07.1, SALADO, PKG#19, ROCK COMPRESS. | IP | YES | SWCF-A/SAIC | X |
| 33 | 31217 | DOMSKI, P.S. | SALADO | ANHYDRITE PERMEABILITY | PDD, 1.2.07.1, SALADO, PKG#13, ANHYD. PERM. | IP | YES | SWCF-A/SAIC | X |
| 34 | 31218 | DOMSKI, P.S. | SALADO | HALITE PERMEABILITY | PDD, 1.2.07.1, SALADO, PKG#7 HALITE PERM (X, Y, Z) | IP | YES | SWCF-A/SAIC | X |
| 35 | 31220 | DOMSKI, P.S. | SALADO | HALITE ROCK COMPRESSIBILITY | PDD, 1.2.07.1, SALADO, PKG#5 HALITE ROCK COMP. | IP | YES | SWCF-A/SAIC | X |
| 36 | 31221 | DOMSKI, P.S. | SALADO | HALITE PRESSURE | PDD, 1.2.07.1, SALADO, PKG#4, HALITE PRESSURE | IP | YES | SWCF-A/SAIC | X |
| 37 | 32032 | DOMSKI, P.S. | SALADO | GAS-THRESHOLD PRESSURE | PDD, 1.2.07.1, SALADO PKG#10 | IP | YES | SWCF-A/SAIC | X |
| 38 | 32033 | DOMSKI, P.S. | SALADO | TRANSITION ROCK COMPRESSIBILITY | PDD, 1.2.07.1, SALADO PKG#16 | IP | YES | SWCF-A/SAIC | X |
| 39 | 32034 | DOMSKI, P.S. | SALADO | TRANSITION PERMEABILITY | PDD, 1.2.07.1, SALADO PKG#16 (X, Y, Z) | IP | YES | SWCF-A/SAIC | X |
| 40 | 32035 | DOMSKI, P.S. | SALADO | TRANSITION PRESSURE | PDD, 1.2.07.1, SALADO PKG#16 TRAN. PRES | IP | YES | SWCF-A/SAIC | X |
| 41 | 32036 | DOMSKI, P.S. | SALADO | DRZ PRESSURE | PDD, 1.2.07.1, SALADO PKG#16 DRZ | IP | YES | SWCF-A/SAIC | X |
| 42 | 32037 | DOMSKI, P.S. | SALADO | DRZ ROCK COMPRESSIBILITY | PDD, 1.2.07.1, SALADO PKG#16 DRZ ROCK. COMP. | IP | YES | SWCF-A/SAIC | X |
| 43 | 32038 | DOMSKI, P.S. | SALADO | DRZ PERMEABILITY | PDD, 1.2.07.1, SALADO PKG#16 DRZ PERM. (X, Y, Z) | IP | YES | SWCF-A/SAIC | X |
| 44 | 35193 | RUSKAUFF, G. | NON-SALADO | CULEBRA TRANSMISSIVITY FIELD INDEX | PDD, 1.2.07, NON-SALADO CULEBRA TRANS. | IP | NO | SWCF-A/SAIC | X |
| 45 | 35194 | WEINER, R. | MISC. | OXIDATION STATE DISTRIBUTION | PDD, 1.1.10.1.1, OXIDATION STATE | IP | YES | SWCF-A/SAIC | |
| 46 | 35406 | BEAUHEIM, R. | NON-SALADO | CULEBRA TRANSMISSIVITY DATA | PDD, 1.2.07.1, TRANSMISSIVITY DATA | IP | YES | SWCF-A/SAIC | X |
| 47 | 35695 | BUTCHER, B. | MISC. | CUTTINGS RELEASE OF SOLIDS CAUSED BY BLOWOUT | PDD, 1.1.01.1.5, CUTTINGS' | IP | YES | SWCF-A/SAIC | |
| 48 | 35697 | BUTCHER, B. | MISC. | FINAL POROSITY SURFACE DATA | PDD, 1.1.01.2.3, POROSITY SURFACE DATA | IP | YES | SWCF-A/SAIC | |
| 49 | 35835 | SIEGEL, M. | MISC. | SOLUBILITY PARAMETERS FOR ACTINIDE SOURCE TERM LOOK-UP TABLES | PDD, 1.1.10.1, ACTINIDE SOLUBILITY TABLES | IP | YES | SWCF-A/SAIC | |
| 50 | 35843 | BEAUHEIM, R. | NON-SALADO | CULEBRA FLUID-DENSITY DATA | PDD, 1.2.07.1, CULEBRA FLUID-DENSITY DATA | IP | YES | SWCF-A/SAIC | |
| 51 | 35850 | PAPENGUTH, H. | MISC. | MOBILE-COLLOIDAL-ACTINIDE SOURCE TERM 1. MINERAL FRAGMENT COLLOIDS | PDD, 1.1.10.2.1, MINERAL FRAGMENT COLLOIDS | IP | YES | SWCF-A/SAIC | |
| 52 | 35852 | PAPENGUTH, H. | MISC. | MOBILE-COLLOIDAL-ACTINIDE SOURCE TERM 2. ACTINIDE INTRINSIC COLLOIDS | PDD, 1.1.10.2.1, ACTINIDE INTRINSIC COLLOIDS | IP | YES | SWCF-A/SAIC | |
| 53 | 35855 | PAPENGUTH, H. | MISC. | MOBILE-COLLOIDAL-ACTINIDE SOURCE TERM 3. HUMIC SUBSTANCES | PDD, 1.1.10.2.1, HUMIC SUBSTANCES | IP | YES | SWCF-A/SAIC | |
| 54 | 35856 | PAPENGUTH, H. | MISC. | MOBILE-COLLOIDAL-ACTINIDE SOURCE TERM 4. MICROBES | PDD, 1.1.10.2.1, MICROBES | IP | YES | SWCF-A/SAIC | |
| 55 | 36425 | CORBET, T. | NON-SALADO | CLIMATE INDEX | PDD, TBD, CLIMATE INDEX | IP | YES | SWCF-A/SAIC | X |
| 56 | 36453 | WANG, Y. | MISC. | DEFINE REPOSITORY CHEMISTRY FOR THE LONG-TERM WIPP PERFORMANCE ASSESSMENT | PDD, 1.1.09.1.1, REPOSITORY CHEMISTRY | IP | YES | SWCF-A/SAIC | |
| 57 | 36455 | BEAUHEIM, R. | NON-SALADO | CULEBRA THICKNESS DATA | PDD, 1.2.07.1, CULEBRA THICKNESS DATA | IP | YES | SWCF-A/SAIC | X |
| 58 | 36456 | BEAUHEIM, R. | NON-SALADO | CULEBRA STORATIVITY DATA | PDD, 1.2.07.1, STORATIVITY DATA | IP | YES | SWCF-A/SAIC | X |

## Table 10. Listing of PI Parameter Packages (concluded)

| # | WPO# | PI/SOURCE OF PRP | GROUP | TITLE OF PARAMETER RECORD PACKAGE (PRP) | FILE CODE OF PRP IN AIMS DATABASE-PDD, WBS#, PKG IDENTIFIER | STATUS | W/DATA | DUAL STORAGE | AIMS TABLE OF CONTENTS |
|---|---|---|---|---|---|---|---|---|---|
| 59 | 36489 | WALLACE, M. | NON-SALADO | MINING TRANSMISSIVITY MULTIPLIER | PDD, 1.2.07.1, MINING MULTIPLIER | IP | YES | SWCF-A/SAIC | X |
| 60 | 36491 | WALLACE, M. | MISC. | SKIN RESISTANCE | PDD, 1.2.07.1, SKIN RESISTANCE | IP | YES | SWCF-A/SAIC | |
| 61 | 36548 | BUTCHER, B. | MISC. | INITIAL WASTE WATER CONTENT | PDD, 1.2.07.1, INITIAL WASTE WATER CONTENT | IP | YES | SWCF-A/SAIC | |
| 62 | 36549 | BUTCHER, B. | MISC. | WASTE PERMEABILITY | PDD, 1.2.07.1, WASTE PERMEABILITY | IP | YES | SWCF-A/SAIC | |
| 63 | 37223 | MEIGS, L. | NON-SALADO | CULEBRA EFFECTIVE THICKNESS | PDD, 1.2.07.1, EFFECTIVE THICKNESS | IP | YES | SWCF-A/SAIC | X |
| 64 | 37225 | MEIGS, L. | NON-SALADO | CULEBRA HALF MATRIX BLOCK LENGTH | PDD, 1.2.07.1, HALF MATRIX | IP | YES | SWCF-A/SAIC | |
| 65 | 37226 | MEIGS, L. | NON-SALADO | CULEBRA DIFFUSIVE TORTUOSITY | PDD, 1.2.07.1, DIFFUSIVE TORTUOSITY | IP | YES | SWCF-A/SAIC | X |
| 66 | 37227 | MEIGS, L. | NON-SALADO | CULEBRA ADVECTIVE POROSITY | PPD, 1.2.07.1, ADVECTIVE POROSITY | IP | YES | SWCF-A/SAIC | |
| 67 | 37228 | MEIGS, L. | NON-SALADO | CULEBRA DIFFUSIVE POROSITY | PDD, 1.2.07.1, DIFFUSIVE POROSITY | IP | YES | SWCF-A/SAIC | |
| 68 | 37230 | MCCORD, J. | NON-SALADO | CULEBRA LONGITUDINAL DISPERSIVITY | PDD, 1.2.07.1, LONGITUDINAL DISPERSIVITY | IP | YES | SWCF-A/SAIC | |
| 69 | 37231 | MCCORD, J. | NON-SALADO | RATIO OF LONGITUDINAL TO TRANSVERSE DISPERSIVITY FOR THE CULEBRA | PDD, 1.2.07.1, RATIO OF LONGITUDINAL | IP | YES | SWCF-A/SAIC | |
| 70 | 37232 | MEIGS, L. | NON-SALADO | CULEBRA GRAIN DENSITY | PDD, 1.2.07.1, GRAIN DENSITY | IP | YES | SWCF-A/SAIC | |
| 71 | 37287 | BEAUHEIM, R. | NON-SALADO | CULEBRA TRANSIENT POINT PRESSURE DATA | PDD, 1.2.07.1, TRANSIENT POINT | IP | YES | SWCF-A/SAIC | |
| 72 | 37288 | BEAUHEIM, R. | NON-SALADO | CULEBRA STEADY STATE FRESHWATER HEADS | PDD, 1.2.07.1, FRESHWATER HEADS | IP | YES | SWCF-A/SAIC | X |
| 73 | 38173 | PAPENGUTH, H. | MISC. | COLLOIDAL ACTINIDE RETARDATION PARAMETERS | PDD, 1.1.10.2.1, COLLOIDAL ACTINIDE RETARDATION | IP | YES | SWCF-A/SAIC | |
| 74 | 38231 | BRUSH, L. | MISC. | CULEBRA DISSOLVED ACTINIDE DISTRIBUTION COEFFICIENTS (KD'S) | PDD, 1.1.10.3.1, DISTRIBUTION COEFFICIENTS | IP | YES | SWCF-A/SAIC | |
| 75 | 38304 | MCCORD, J. | NON-SALADO | MULTIPHASE FLOW PARAMETERS | PDD, 1.2.07.1, MULTIPHASE FLOW PARAMETERS | IP | YES | SWCF-A/SAIC | |
| 76 | 38344 | HOWARTH, S. | MISC. | NOMINAL WELLBORE DIAMETER | PDD, 1.2.07.1, BOREHOLE DIAMETER | IP | YES | SWCF-A/SAIC | |
| 77 | 39571 | BRUSH, L. | MISC. | CULEBRA FREE-SOLUTION TRACER DIFFUSION COEFFICIENTS (Dsols) | PDD, 1.1.10.3.1, CULEBRA FREE-SOLUTION | IP | YES | SWCF-A/SAIC | |
| 78 | 39622 | CHU, M. | MISC. | PERMEABILITY OF BOREHOLE WITH CREEP CLOSURE | PDD, 1.2.07.1, CREEP CLOSURE | IP | YES | SWCF-A/SAIC | |
| 79 | 39624 | CHU, M. | MISC. | PERMEABILITY OF BOREHOLE WITH SURFACE AND RUSTLER CONCRETE PLUG | PDD, 1.2.07.1, CONCRETE PLUG | IP | YES | SWCF-A/SAIC | |
| 80 | 39626 | CHU, M. | MISC. | PERMEABILITY OF BOREHOLE FILLED WITH SILTY SAND | PDD, 1.2.07.1, SILTY SAND | IP | YES | SWCF-A/SAIC | |
| 81 | 40199 | CHU, M. | MISC. | PROBABILITY OF INTERCEPTING A PRESSURIZED BRINE RESERVOIR UNDER THE WIPP | PDD, 1.2.07.1, BRINE ENCOUNTERS | IP | YES | SWCF-A/SAIC | |
| 82 | 40512 | BYNUM, R. | MISC. | ESTIMATION OF THE UNCERTAINTY FOR PREDICTED ACTINIDE SOLUBILITIES | PDD, 1.1.10.1.1, PREDICTED ACTINIDE SOLUBILITIES | IP | YES | SWCF-A/SAIC | |
| 83 | 41626 | TIERNEY, M. | MISC. | GUIDE TO CCA WIPP PARAMETER DATABASE | PDD, 1.2.07.1.2, CCA WIPP DATABASE | IP | YES | SWCF-A/SAIC | |
| 84 | 42300 | CORBET, T. | MISC. | STRATIGRAPHIC GRIDDING AND ZONE IDENTIFICATION FOR THE 3-D RUSTLER FORMATION HYDROLOGIC MODEL | PDD, 1.2.07.1, STRATIGRAPHIC GRIDDING | IP | YES | SWCF-A/SAIC MAP ROOM | |
| 85 | 42301 | CORBET, T. | MISC. | STRATIGRAPHIC DATA USED FOR THE 3-D RUSTLER FORMATION HYDROLOGIC MODEL | PD, 1.2.07.1, STRATIGRAPHIC DATA | IP | YES | SWCF-A/SAIC MAP ROOM | |
| 86 | 42302 | CORBET, T. | MISC. | SOURCE CODE, INPUT AND OUTPUT FILES, AND GRAPHICAL RESULTS FROM RUSTLER FORMATION HYDROLOGIC MODEL | PDD, 1.2.07.1, INPUT AND OUTPUT FILES | IP | YES | SWCF-A/SAIC | |
| 87 | 42346 | WALLACE, M. | NON-SALADO | FRACTURE TORTUOSITY | PDD, 1.2.07.1, FRACTURE TORTUOSITY | IP | YES | SWCF-A/SAIC | |
| 88 | 43367 | CORBET, T. | NON-SALADO | DEVELOPMENT AND TESTING OF SECOFL3D | PDD, 1.2.07.1, PDD SECOFL3D | IP | YES | SWCF-A/SAIC | |
| 89 | 43367 | CORBET, T. | NON-SALADO | TESTING OF SECOFL3D V.1.9 | PDD, 1.2.07.1, SECOFL3D TESTING V.1.9 | IP | YES | SWCF-A/SAIC | |

#### 6.10.1.2 Contents

The suggested PIPP format outline is contained in Appendix I. The PIPPs were intended to provide a link between the raw data and the parameter distributions used in the CCA PA. The objectives were to provide consistent, traceable links between PA database parameters and data packages in summary format, provide a data and distribution summary, identify the QA status of data and related interpretive codes, and (where applicable) provide a summary on experimental data collection (i.e., method used, assumptions made in testing and interpretation, related references including SAND reports and test plans, related SWCF file codes, etc.).

Because of the complexity and interrelationship of some groups of parameters (e.g., seals, chemistry, disposal room), the PIPP format outline was not followed in all cases. For the large PIPPs, important information is located in the first section or volume of the package. Once located, this information will help guide users through the package.

##### 6.10.1.2.1 Roadmaps to Technical Data Packages

A roadmap to the appropriate supporting Technical Data Packages is contained within the PI Parameter Record Package. The location of the roadmap within the PIPP is identified in the table of contents of the PIPP. In order to save time and effort, especially when trying to navigate through the larger PIPPs (e.g., the 14-volume PIPP for the Seals Program), it is imperative that users locate the roadmap and use it to find the information of interest.

An example of a PIPP is included in Appendix J. The Marker Bed 139 Anhydrite Permeability PIPP includes a roadmap in Record 3. As discussed previously, not all PIPPs are organized in the same manner. Therefore the following three sections are included to aid readers trying to navigate through the complex Shaft Seals and Chemistry packages.

##### 6.10.1.2.2 Shaft Seals Parameters

Because of the large number of shaft seals parameters (over 400), the parameters were developed by subcontractors (i.e., Duke Engineering Services [formerly Intera] and RE/SPEC) under SNL technical direction. For convenience, the Shaft Seals PIPP (WPO#30640) was organized according to the shaft seal material. Each subcontractor was generally responsible for different materials. Therefore the package is divided into three sections: Section I, SNL oversight contribution; Section II, Intera contributions; and Section III, RE/SPEC contributions.

A roadmap was developed for each seal material (idmtrl). These roadmaps are included in the front of the Shaft Seals PIPP in Section I and in each material section. The roadmap for Compacted Crushed Salt is included in Appendix K as an example of the other roadmaps found in the Shaft Seals PIPP. For each parameter (idpram), the roadmaps provide direction to the pertinent section of the package and identify any literature, other reference sources, and supporting data records packages used to develop the parameter. In addition, a separate report (Hurtado et al., 1997) contains specific details regarding the development of the Shaft Seals parameters.

##### 6.10.1.2.3 Chemistry Parameters Involving the Radionuclide Inventory

Parameters based on the WIPP disposal inventory of radionuclides, presented in Revisions 2 and 3 of the TWBIR, are presented in Table 8. Revisions 2 and 3 of the TWBIR may be considered together, since Revision 3 is an addendum to Revision 2 and includes only a few changes to Revision 2 values. The methods used to estimate the anticipated inventory of the WIPP are described in detail in Chapters 1 and 2 of the TWBIR, Revision 2 and are summarized very briefly below.

Data on currently stored inventories (called "stored inventory" in the TWBIR) were obtained from the generating sites (e.g., ORNL, SRS, LANL, etc.). Additional projected inventory includes waste scheduled to be generated between 1995 and 2022 and is scaled to adjust to the design limit of the WIPP repository. The anticipated WIPP inventory is the sum of the stored inventory and the scaled projected inventory. The TWBIR lists the inventory by generator site as well as providing the total inventory. Parameters related to radionuclide quantities (curies) have a constant distribution. Parameters related to other inventoried materials (e.g., ferrous metals, cellulose) have a uniform distribution; for these materials, each site inventory includes a minimum, maximum, and average quantity.

Table 11 includes the radionuclide-related parameters that are taken from a standard table of nuclides and isotopes (Parrington et al., 1996) and those that are defined by 40 CFR Part 191. Radionuclide-related parameters (INVCHD, INVRHD) are the anticipated inventory curies—the activity or radioactivity—of each radionuclide decayed to the year 2033. The activity of a particular isotope is significant to two different aspects of performance assessment: (1) inclusion in the waste unit factor, the normalization factor for the release limits given in 40 CFR 191.13 and 40 CFR Part 191 (Appendix A Table 1) and (2) inclusion in the CCDF.

Table 11. Relationship of Inventory-Related Radionuclide Parameters to the TWBIR and Other Sources

| Parameter Name* | Definition and Source of Parameter Values |
|---|---|
| ATWEIGHT<br>HALFLIFE. | The atomic weight (in atomic mass unit [a. m. u.]) and radiological half-life of the isotope, respectively, as given in the Table of Isotopes. |
| EPAREL | The regulatory release limit for the isotope. |
| WUF | The waste unit factor used in calculating EPAREL. The waste unit factor is the total curie inventory at closure (in units of $10^6$ Ci) divided into the release limit for the particular isotope given in 40 CFR Part 191, Appendix A Table 1. |
| INVCHD<br>INVRHD | The anticipated radionuclide inventories of CH-TRU and RH-TRU, respectively, as given in the TWBIR Revs. 2 and 3, and decayed to 2033. See below for a brief discussion of the TWBIR; see the TWBIR for a complete discussion. |
| VOLCHW<br>VOLRHW | The total anticipated volumes of CH-TRU waste and RH-TRU waste, respectively, as given in the TWBIR Revs. 2 and 3. See below for a brief discussion of the TWBIR; see the TWBIR for a complete discussion. |

*The parameter name implies parameters using all associated material names.

The *waste unit factor* is a function of the total curie quantity, at closure, of all TRU alpha-emitting radionuclides having a half-life of more than 20 years. Sanchez et al. (1996) analyzed the radionuclide inventory from Revision 3 of the TWBIR with respect to these criteria and gave this inventory at closure as $3.44\times10^6$ curies and the waste unit factor as 3.44. With reference to 40 CFR Part 191 (Appendix A Table 1), one EPA unit of waste is therefore 34.4, 344, 3440, or 34,400 curies. Parameters related to radioactivity express the activity of a particular radionuclide in EPA units—the curies of radionuclide divided by the appropriate factor; 99.9% of the contribution to the waste unit factor is captured by Am-241, Pu-238, 239, 240, 242, and Cm-245.

Unlike the waste unit factor, *all* radionuclides are potentially included in a demonstration of compliance and must therefore be considered for inclusion in the *source term* for any CCDF. However, many radionuclides are present in such small quantities that their impact on long-term performance is negligible. The impact of a radionuclide on performance is assessed by comparison with the EPA release limits given in 40 CFR Part 191 (Appendix A Table 1).

Each radionuclide is normalized with respect to its release limit, and the sum of all releases must have less than one chance in ten of exceeding the release limit, and less than one chance in 1,000 of exceeding ten times the release limit. A more complete explanation of these release limits is given in Appendix WCA of the CCA and in Sanchez (1996); a comprehensive discussion of the background for these limits is provided in EPA (1985).

There are three different source terms for WIPP PA for the three different release mechanisms: (1) direct release in material brought to the surface by drilling, caving, and spalling when a waste container has been penetrated directly; (2) direct release to the surface in brine under pressure; and (3) release to the accessible environment in brine that moves through the Culebra aquifer. The three source terms do not include all the same radionuclides. Therefore, although the radioactivity-related parameter names (idpram) are the same (INVCHD, INVRHD), different material names (idmtrl) are used in the three different source terms.

The direct release scenario, which models direct release by drilling (including caving and spalling) using the CUTTINGS_S code, incorporates the probability of penetrating each of the 569 contact-handled transuranic (CH-TRU) waste streams and the remote-handled transuranic (RH-TRU) waste stream in the CCDF calculation (Sanchez et al., 1996), thereby effectively using waste-stream-level data. Scenarios in which radionuclides would be released in brine, either directly to the surface or through the Culebra aquifer, utilize the total inventory of each applicable radionuclide rather than the inventory of that nuclide in any particular waste stream. Thus the PANEL and NUTS codes use the total inventory of the particular radionuclides instead of waste-stream-level data. The difference is discussed in greater detail in Appendix WCA of the CCA. Discussions of the scaling of the stored waste inventory to WIPP capacity and of the renormalization of the waste stream data are in the TWBIR, Revision 3.

Figure 12 shows how data reported by the generator sites are decayed and grown in to the year 1995. These data are then scaled up to the capacity of the WIPP and used in performance assessment. Data for individual waste streams are renormalized and rolled up to site-level data. Waste stream level data are derived from this roll-up and used in performance assessment to calculate direct release.

#### 6.10.1.3.2 Chemistry Parameters Involving Gas Generation, Colloids, and $K_d$

The brief explanations that follow discuss, in turn, parameters related to gas generation, to retardation and distribution constants, to colloids, and to actinide solubility. Explanations of the use of all these parameters in performance assessment may be found in Appendices SOTERM and WCA of the CCA, and in the Analysis Packages for the codes CUTTINGS_S, PANEL, and NUTS.

Parameters Related to Gas Generation

The processes that can generate gas in the repository are corrosion of ferrous and nonferrous metals and microbial metabolism that produces $CO_2$ and $CH_4$. Parameters listed in Table 12 are used as indicated to calculate gas generation from metal corrosion and from metabolism of carbon-containing compounds. The estimated inventories of nitrate and sulfate (QINIT NITRATE, QINIT SULFATE) are used to calculate $CO_2$ production. These processes are discussed in detail in Appendix SOTERM of the CCA and in Wang and Brush (1996). Inventories of ferrous metals and of cellulosics, plastics, and rubber are also used in these calculations. These inventories were developed as described in the TWBIR, Rev. 2, Chapters 2 and 3. Information from the generating sites provided uniform distributions for parameters related to inventories. The inventoried amount of cementitious waste (containing calcium oxide) was calculated to be insufficient to affect pH or brine composition significantly (Wang, 1996).

The initial water content of the waste is important with regard to estimating gas generation rates with the BRAGFLO code because it defines how much brine is immediately available for the corrosion reaction. However, based on waste characterization data and transportation restrictions on the amount of free liquid that the waste can contain, the liquid in the waste is negligible compared to brine.

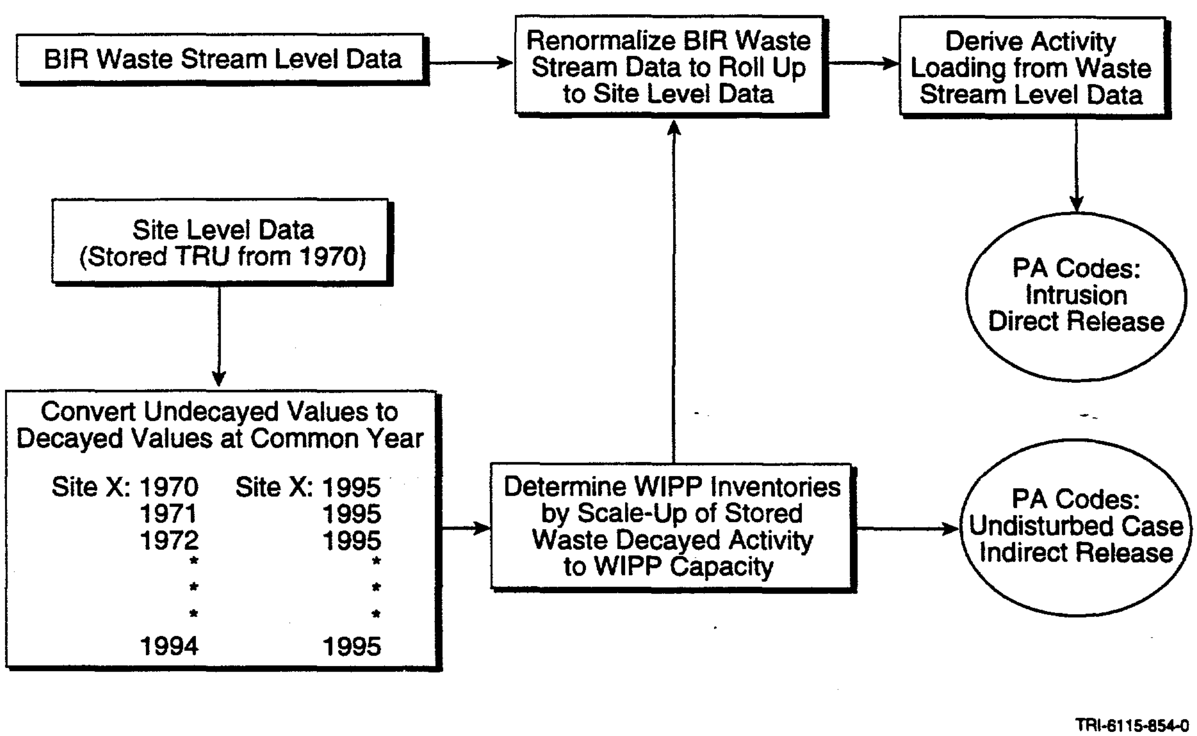


Figure 12. Flow chart for inventory input into performance assessment (after Figure WCA-2, Appendix WCA, Section WCA.2.1 of DOE, 1996).

Table 12. Parameters Related to Gas Generation

| Parameter Name* | Definition and Source of Parameter Values |
|---|---|
| ASDRUM | Surface area of corrodable metal per drum. Ferrous metal inventories are given in the TWBIR Revs. 2 and 3. See below for a brief discussion of the TWBIR; see the TWBIR for a complete discussion. |
| QINIT | Initial quantity of sulfates, nitrates, phosphates, etc. in the waste, as given in the TWBIR Rev. 3, Appendix B-6 |
| VOLCHW<br>VOLRHW | The total anticipated volumes of CH-TRU waste and RH-TRU waste, respectively, as given in the TWBIR Revs. 2 and 3. See below for a brief discussion of the TWBIR; see the TWBIR for a complete discussion. |
| **Material and Parameter Name** | |
| STEEL STOIFX<br>STEEL CORRMCO2 | Uniformly distributed parameters for the corrosion of ferrous metal (including containers) in the anticipated waste inventory in the absence of carbon dioxide, under inundated conditions. STOIFX is a stoichiometric constant. |
| STEEL STOIFX<br>STEEL HUMCOR | Uniformly distributed parameters for the corrosion of ferrous metal (including containers) in the anticipated waste inventory under humid conditions. |
| WAS_AREA GRATMICI<br>WAS_AREA GRATMICH | The rate of microbial degradation of the anticipated waste inventory of cellulose under inundated and humid conditions, respectively. These parameters are uniformly distributed. |
| WAS_AREA PROBDEG | The probability of microbial degradation of the anticipated waste inventory of plastics and rubber in the waste (including liners); a delta distribution |

*The parameter name implies parameters using all associated material names.

#### Parameters Related to Retardation

Retardation depends on experimental determination of an applicable range of partition coefficient ($K_d$) values and on the oxidation state of the actinide element under consideration, and not on inventory values. Three of the four actinides under consideration—uranium, neptunium, and plutonium—each have two possible oxidation states and are considered to be present half the time in each of the two states, as indicated by the parameter OXSTAT. Uranium can be either +4 or +6; plutonium can be +3 or +4; neptunium can be +4 or +5. Thorium is always in the +4 oxidation state, and americium is in the +3 oxidation state. Complete discussions of the experimental data developed for each of these actinides are found in WPO#38231 for $K_d$ values, in WPO#35194 for the oxidation state distribution of the actinides, and in Appendix SOTERM of the CCA. Table 13 provides definitions and sources for the parameters related to retardation.

#### Parameters Related to Colloids

Colloid related parameters express the results of the colloidal actinide investigations and were conveyed to performance assessment in three types of parameter values: (1) constant concentration values for actinides associated with mineral fragment and actinide intrinsic colloids; (2) concentration values proportional to the dissolved actinide concentration for actinides associated with microbes and humic substances; and (3) maximum concentration values providing an upper limit for actinide concentrations associated with microbes and humic substances.

Table 13. Definition and Sources of Retardation Parameter Values

| Parameter Name* | Definition and Source of Parameter Values |
|---|---|
| MKD_U | Matrix partition coefficient for uranium; parameters include appropriate oxidation states of uranium. Uniformly distributed. |
| MKD_PU | Matrix partition coefficient for plutonium; parameters include appropriate oxidation states of plutonium. Uniformly distributed. |
| MKD_TH | Matrix partition coefficient for thorium; parameters include appropriate oxidation states of thorium. Uniformly distributed. |
| MKD_AM | Matrix partition coefficient for americium; parameters include appropriate oxidation states of americium. Uniformly distributed. |
| MKD_NP | Matrix partition coefficient for neptunium; parameters include appropriate oxidation states of neptunium. Uniformly distributed. |
| OXSTAT | Parameter indicating whether an actinide is in the higher or lower of two possible oxidation states. A delta distribution. |

*The parameter name implies parameters using all associated material names.

The parameter values are not derived directly from the waste inventory. A detailed discussion can be found in the parameter record packages describing the determination of the mobile colloidal actinide source term (Papenguth, 1996b, c, d; Papenguth and Moore, 1996) as well as in Appendices SOTERM and WCA of the CCA. Table 14 contains material and property names for parameters related to colloids.

Table 14. Material and Parameter Names for Colloids

| IDMTRL | IDPRAM | Brief Description of Parameter |
|---|---|---|
| Th, U, Np, Pu, Am | CONCMIN | Concentration of actinide associated with mobile mineral fragment colloids |
| Th, U, Np, Pu, Am | CONCINT | Concentration of actinide associated with mobile actinide intrinsic colloids |
| Th, U, Np, Pu, Am | PROPMIC | Proportionality constant for concentration of actinides associated with mobile microbes. |
| PHUMOX3*<br>PHUMOX4<br>PHUMOX5<br>PHUMOX6 | PHUMCIM | Proportionality constant for concentration of actinides associated with mobile humic colloids, in Castile brine; actinide solubilities are inorganic only (complexes with manmade organic ligands are not important); solubilities were calculated assuming equilibrium with Mg-bearing minerals (brucite and magnesite). |
| PHUMOX3*<br>PHUMOX4<br>PHUMOX5<br>PHUMOX6 | PHUMSIM | Proportionality constant for concentration of actinides associated with mobile humic colloids, in Salado brine; actinide solubilities are inorganic only (complexes with manmade organic ligands are not important); solubilities were calculated assuming equilibrium with Mg-bearing minerals (brucite and magnesite). |
| Th, U, Np, Pu, Am | CAPMIC | Maximum (cap) concentration of actinide associated with mobile microbes. |
| Th, U, Np, Pu, Am | CAPHUM | Maximum (cap) concentration of actinide associated with mobile humic colloids. |

*Proportionality constant for concentration of actinides associated with mobile humic substances, for PHUMOX3, actinide elements with oxidation state 3 [i.e., Pu(III) and Am(III)]; PHUMOX4, oxidation state 4 [i.e., Th(IV), U(IV), Np(IV), and Pu(IV)]; PHUMOX5, oxidation state 5 [i.e., Np(V)]; PHUMOX6, and oxidation state 6 [i.e., U(VI)].

Parameters Related to Actinide Solubility

A complete discussion of actinide solubility parameters and how they are used in performance assessment is found in Section 7 of Appendix SOTERM of the CCA and in the Analysis Packages for the codes PANEL and NUTS. The parameter and material names are listed in Table 15. These parameters were addressed in performance assessment somewhat differently from other parameters. The parameter OXSTAT determines whether an actinide that can exhibit two oxidation states is in the higher or lower oxidation state. The values of the parameters SOLMOD*X* SOLCIM and SOLMOD*X* SOLSIM, where *X* takes the values 3, 4, 5, and 6, are the values of the solubility of the +3, +4, +5, and +6 actinide analogues, respectively, in Castile brine at pH 9.9, and in Salado brine at pH 9.4, as modeled by the FMT code. These parameters are single-valued functions and are tabulated in Appendix SOTERM. The parameters SOL*ANX* SOLCIM and SOL*ANX* SOLSIM, where *AN* symbolizes AM, PU, U, TH, and NP, are sampled from the logcumulative uncertainty distribution around SOLMOD*X* SOLCIM and SOLMOD*X* SOLSIM, the modeled solubilities. SOL*ANX* SOLCIM and SOL*ANX* SOLSIM can take values from -2 to +1.4 (i.e., the modeled solubility is multiplied by a sampled number between $10^{-2}$ and $10^{1.4}$). The solubility of an actinide in Castile brine is given by the expression

$$\text{Solubility} = \text{SOLMOD}X\ \text{SOLCIM} \times 10^{\text{SOLANX SOLCIM}}$$

and in Salado brine by

$$\text{Solubility} = \text{SOLMOD}X\ \text{SOLSIM} \times 10^{\text{SOLANX SOLSIM}}$$

so that, for example, the solubility of plutonium in the +4 oxidation state in Salado brine is given by

$$\text{Solubility of Pu } (+4) = \text{SOLMOD4 SOLSIM} \times 10^{\text{SOLPU4 SOLSIM}}$$

This solubility is then used in performance assessment.

Note that dissolution of the actinides may be enhanced directly by the formation of soluble complexes, including chelates. As shown in the TWBIR, Rev. 3, the waste contains complexing agents soluble in aqueous media that might have an impact on performance. Four of these complexants are present in the waste in nonnegligible quantities: acetate, citrate, oxalate, and ethylene diamine tetra-acetate (EDTA).

These complexants have the potential for increasing the dissolution of metal ions when compared to the inorganic system in the absence of organic ligands. The effect of these complexants on the solubility of actinides in both Salado and Castile brines has been studied and is discussed in detail in Appendix SOTERM of the CCA; it was initially expressed by parameters SOLSOM (Salado brine with organic complexants) and SOLCOM (Castile brine with organic complexants). However, modeling predicts that for the amount of these complexants expected to be emplaced in the repository, as reflected in the inventory, the concentration of americium and plutonium in solution are increased by very small amounts, and the complexants are expected to bind preferentially to nonactinide metal species in the waste, including iron (Fe), nickel (Ni), chromium (Cr), vanadium (V), and manganese (Mn). Based on the inventory of drum and waste boxes, the amount of these metals expected to be emplaced is more than enough to sequester the organic complexants. Hence there are no parameters for organic complexants.

Table 15. Material and Parameter Names for Actinide Solubility Parameters

| Parameter Name | Definition and Source of Parameter Values |
|---|---|
| SOLSIM | Parameter indicating dissolution in Salado brine, no organic material. Source is the FMT model (WPO #35835). |
| SOLCIM | Parameter indicating dissolution in Castile brine, no organic material. Source is the FMT model (WPO #35835). |
| OXSTAT | Parameter indicating whether an actinide is in the higher or lower of two possible oxidation states. A delta distribution. |
| **Material and Parameter Name** | |
| SOLAM3 | Parameter indicating uncertainty distribution of solubility of americium in the +3 oxidation state. |
| SOLPU3 | Parameter indicating uncertainty distribution of solubility of plutonium in the +3 oxidation state. |
| SOLPU4 | Parameter indicating uncertainty distribution of solubility of plutonium in the +4 oxidation state. |
| SOLU4 | Parameter indicating uncertainty distribution of solubility of uranium in the +4 oxidation state. |
| SOLTH4 | Parameter indicating uncertainty distribution of solubility of thorium in the +4 oxidation state. |
| SOLU6 | Parameter indicating uncertainty distribution of solubility of uranium in the +6 oxidation state. |
| SOLNP4 | Parameter indicating uncertainty distribution of solubility of neptunium in the +4 oxidation state. |
| SOLNP5 | Parameter indicating uncertainty distribution of solubility of neptunium in the +5 oxidation state. |
| SOLMOD3 | Parameter indicating FMT-modeled solubility of an actinide in the +3 oxidation state. |
| SOLMOD4 | Parameter indicating FMT-modeled solubility of an actinide in the +4 oxidation state. |
| SOLMOD5 | Parameter indicating FMT-modeled solubility of an actinide in the +5 oxidation state. |
| SOLMOD6 | Parameter indicating FMT-modeled solubility of an actinide in the +6 oxidation state. |
| **Material and Parameter Name** | |
| CS LOGSOLM | Parameter for the log of the solubility of cesium (constant). |
| RA LOGSOLM | Parameter for the log of the solubility of radium (constant). |
| SR LOGSOLM | Parameter for the log of the solubility of strontium (constant). |

### 6.10.2 Category 2

As described in detail in Section 4.2.3, many of the Category 2 parameters were derived from the TWBIR (DOE, 1995-1996). These parameters were the responsibility of the PA Analysts. The "Source" block of Form 464 contains references to the supporting documentation for Category 2 parameters. Additional information is found in Appendix SOTERM of the CCA and in Section 4.2.3 above.

### 6.10.3 Category 3

Parameters whose source information can be found in technical literature and scientific handbooks, or which are based on general engineering or scientific knowledge, comprise the Category 3 subgroup. These parameters are constants and the responsibility of the PAAs. For these parameters, the information from the source was entered into Form 464 and a citation reference was included on Form 464. A copy of the page from the source document was stapled to Form 464 to complete the PRP. If some type of minor calculation was required (e.g., unit conversion) the PRP also contained the calculation and the signature of the person who performed the technical review of the calculation per SNL QAP 9-5.

### 6.2.10.4 Category 4a

Category 4a parameters are analogues, and supporting information may be linked back to Category 1 parameters or other supporting information. For example, the log of the permeability of Salado anhydrite layers a and b is analogued to Salado Marker Bed 139, for which experimental data were available. In this case, Salado Marker Bed 139 is a Category 1 parameter and Salado anhydrite layers a and b are category 4a parameters. Category 4a parameters are "co-owned" by the PAA and PIs. Concurrence is required of the PI, PAA, and PTL for Category 4a parameters.

As described in Section 4.2.5, documentation of the development of Category 4a parameters is contained in the PRP (see Section 7) and referenced in the "Source" block of Form 464 or in the PA Code Analysis Packages. Because the PA Code Analysis Packages were not complete at the time the Form 464s were completed and used, there is no direct link to these analysis packages on Form 464. A listing of the PA Code Analysis Packages and the WPO number of each is contained is Table 3.

### 6.2.10.5 Category 4b

Category 4b parameters are primarily model configuration parameters. These parameters are "owned" by the PAA. Concurrence on Form 464 is required of the PAA and PTL for all Category 4b parameters.

As described in Section 4.2.6, documentation of the development of Category 4b parameters is contained in the PRP (see Section 7) and referenced in the "Source" block of Form 464 or in the PA Code Analysis Packages. Because the PA Code Analysis Packages were not complete at the time the Form 464s were completed and used, there is no direct link to these analysis packages on Form 464. A listing of the PA Code Analysis Packages and the WPO number of each is found is Table 3.

Memoranda are included or referenced within the PRP for the parameters that identify the WPO number for the appropriate analysis package (see Table 3). Because the code analysis packages had not completed final review and publication at the time the CCA codes were run, according to QAP 9-2 they could not be referenced directly as a source on Form 464.

To provide a direct link from the PRP to the analysis packages, a memorandum was written documenting which parameters were addressed in which analysis packages; this memo was placed in the correspondence file (in the SWCF) for the PRPs and is included in Appendix E of this report. A second link was provided by the inclusion of a reference to the WPO number of the analysis packages in the "Additional Sources" table of the EPA Parameter Database, which identifies Technical Traceability Documents (see Section 8 and Appendix M2).

#### 6.2.10.5.1 Category 4b Legacy and Placeholder Parameters

As described in Section 4.2.7, two groups of Category 4b parameters fell outside the bounds of QAP 9-2: legacy and placeholder parameters. Legacy parameters are those that had the same values or distributions as in the 1992 PA or in other calculations run prior to the CCA calculations. Placeholder parameters are those that are required to run the code but have no effect on the calculation.

Because they were exempt from QAP 9-2 (which covers "new" and "modified" parameters as they relate to the 1992 PA), parameter development and citations of source information for the legacy parameters are found in the 1992 PA documentation or in earlier documents. The QAP 9-2 and Form 464 process did not exist prior to the CCA (1996), and no form resembling Form 464 existed for parameters in the 1992 PA.

Later, as a result of audits, surveillances, and technical reviews, it became apparent that the completion of a Form 464 for each parameter, including legacy and placeholder parameters, would be helpful for tracing parameter information in a manner consistent with the other parameters. The legacy and placeholder parameters were carefully reviewed by the appropriate PIs and PAAs: All were reclassified as Category 4b and a Form 464 was filled out for each and filed in the SWCF. Although not specifically required by QAP 9-2, all parameters in the CCA PA Parameter Database now have an associated Form 464.

Documentation of the development of Category 4b parameters, including legacy and placeholder parameters, is contained in the PRP (see Section 7), referenced in the "Source" block of Form 464, or included in the PA Code Analysis Packages (see Section 4.2.7.1). A listing of the PA Code Analysis Packages and the WPO number of each is found is Table 3.

To provide a direct link from the PRP to the analysis packages, a memorandum was written documenting which parameters were addressed in which analysis packages; this memorandum was placed in the correspondence file (in the SWCF) for the PRPs and is included in Appendix E. In addition to the information related to all 4b parameters contained in Appendix E, Appendix F contains three memoranda related to the legacy and placeholder parameters.

The first memorandum was from Tierney and Vaughn to File, dated June 17, 1996: "Designation of 'Legacy Parameters' and 'Placeholders' in the WIPP Parameter Database." This memorandum lists many legacy and placeholder parameters. During the parameter and CCA review, it was found to be incomplete.

The second memorandum in Appendix F (Martell to Memo of Record, dated February 27, 1997: "Addenda to WPO#38568 SNL Internal Memo: M. Tierney and P. Vaughn to File 6/17/96, Designation of 'Legacy Parameters' and 'Placeholders' in the WIPP Parameter Database") was written to clarify the information found in the first memorandum. It also provided a complete list of the legacy and placeholder parameters.

The third memorandum (Martell and Howarth to Memo of Record dated September 2, 1997: "Addenda to 'Legacy Parameter' memorandum WPO#44202") was written to explain and document the rationale for placing legacy and placeholder parameters in the 4b category.

## 6.11 Interpretation

This field of Form 464 generally contains notes or other information to document or clarify assumptions used by the PTL when developing the parameter or distribution. It may include discussions related to the selection of a parameter value, range, or distribution type different from the one recommended by the PI or PAA.

## 6.12 Miscellaneous

The four check boxes near the top of Form 464 are used to indicate major modifications, error corrections, new parameters, or deactivation. Each box checked results in the following actions.

*Major Modification*: input the information on Form 464 into the database.

*Error Correction*: enter the correct information into the database as found on Form 464.

*New*: create a new id number and input the information into the database.

*Deactivation*: change the parameter's database information (e.g., category=5, active =N, update the data and data entry personnel).

In the *Attachment* box, "yes" is marked if the attachment pertains to either the distribution, interpretation, or source. In some cases, the attachment is a single writeup that addresses both areas. If both *Attachment* boxes are marked "yes" this does not imply that there are two separate attachments.

The *Qualified Parameter* box is not used (see QAP 9-2 Revision 2) but is present on older Form 464s.

The *Entered by* field contains the name and signature of the data entry person.

The *Entry Checked by* field contains the signature of the person who checked that the data were correctly entered.

Some additional notes regarding data entry and check signature dates follow:

As required by QAP 9-4, the data entry must be checked, and both the data entry person and the checker must sign and date Form 464. According to the procedure, the data are first entered and then checked for errors. If an error is found, the form is returned to the data entry person for correction. When the checker is satisfied that the data were correctly entered, the checker signs and dates Form 464. The signed form is then returned to the data entry person for signature and date.

As data were entered to the CCA database using Form 464, the form was revised, as described below, to allow for changes resulting from the concurrent evolution of the parameter development process and the associated QAPs.

1. QAP 9-2 did not define "qualified" parameters. As a result, the use of the *Qualified Parameter* box on earlier Form 464s was nullified. All parameters used in the CCA are qualified because they were developed under the SNL QA program.

2. After an internal audit was conducted, it was determined that QAP 9-5 should be applied to the calculation of distributions for some parameters. All Form 464s were subsequently reviewed to determine whether a technical review was necessary. The distribution calculations were technically reviewed when required.
3. A change in parameter category from 1 to any other category was determined to be a "major modification." Such a change requires the application of QAP 9-2 and the use of Form 464.

## 6.13 Request Memoranda

According to QAP 9-2, the PAA is required to document in a request memorandum the need and intended use for a parameter. The request memorandum is to be submitted to the PTL for approval. Appendix L contains a Memorandum of Record from Susan Pickering, dated September 16, 1996: "Request, Intended Use and Rationale for Major Modifications for Parameter Values Used in Support of the CCA Calculation." This memorandum contains a cross-reference from the parameter type (defined by the experimental program that generated supporting data) to the WPO number of the document that contains the need and intended use of the parameter.

## 6.14 Concurrence

For Category 1 and 4a parameters, concurrence signatures are required for the PTL, PI and PAA. For Category 2, 3, and 4b parameters, concurrence signatures are required for the PAA and the PTL.

If the parameter is a category 1 or a 4a, the PTL and the PAA meet with the appropriate PI, who assembles a PIPP. Once the PI assembles a PIPP, it is provided to the PTL. The PTL then determines the appropriate parameter distribution and completes Form 464. The PTL or designee then signs Form 464 and passes it to the PI and the PAA. If the PI and PAA concur with the distribution values selected, they also sign Form 464. If the PI and PAA do not concur, a dispute-resolution meeting is convened and the PI, PAA, and PTL establish a mutually agreeable parameter distribution. Note that concurrence by the PI is only required for Category 1 and 4a parameters.

# 7. Parameter Traceability and Retrieveability

The CCA probability models require input parameters that are defined by a statistical distribution. Developing parameters begins with the assignment of an appropriate distribution type, which is dependent on the type, magnitude, and volume of data or information available. Parameter development may require interpretation or statistical analysis of raw data, combining raw data with literature values, scaling laboratory or field data to fit code grid mesh sizes, or other transformations. Documentation of parameter development is designed to answer two questions: "*What* source information was used to develop this parameter?" and "*Why* was this particular data set/information used?" Therefore, complete documentation requires integrating information from code sponsors, PTLs, PAAs, and experimental PIs.

Ideally, a user would be able to trace from the parameter information contained in the CCA PA Parameter Database to supporting information using only the information contained in the PRP, as described below in Section 7.1. After submitting the CCA to the EPA it was apparent that in most cases the PIs could trace parameter information from the PA Parameter Database to the supporting information. However, independent reviewers (EPA staff, QA auditors, and some SNL technical staff), not familiar with the work, experienced difficulty in tracing supporting parameter information. Based on the difficulty experienced by the independent reviewers, it was recognized that there was a need for additional supporting documentation, ties to additional supporting information, and/or clarification for many parameters. The additional information was documented in memoranda and in a database created from the WIPP CCA PA Parameter Database specifically for the post-CCA submittal review.

In order to trace through to the source information for a particular parameter, two routes should be followed, as shown in Figure 13. The first route, Track 1, uses information contained in or referenced from the PRP as it existed when the CCA calculations were run. The second route, Track 2, leads from the EPA Parameter Database to additional supporting information. For completeness, users should follow both paths to properly review the information supporting a particular parameter.

As shown in Figure 13, the point of entry to the tracking process is this Parameter Guidebook. Each CCA PA Parameter is uniquely identified three ways: by an identification number, by the WPO number of its Form 464, or by a two-part name consisting of a material name and a parameter name. Appendices in this guidebook contain cross-references of parameter and material names and parameter identification numbers. A parameter's identification number is required to use both tracking systems.

## 7.1 Track 1: Parameter Trace Using the Parameter Records Package System

All references pertaining to the development of a particular parameter are contained within three levels of parameter and data documentation, as shown in Figure 14. After a parameter identification number is known, the PRP may be obtained from the SWCF. The PRP for each parameter includes a Form 464, which contains parameter identification and category, distribution type and values, source references, and additional information such as concurrence and data entry signatures. As illustrated in Figure 14, the number of tiers of supporting information depends on the category of the parameter.

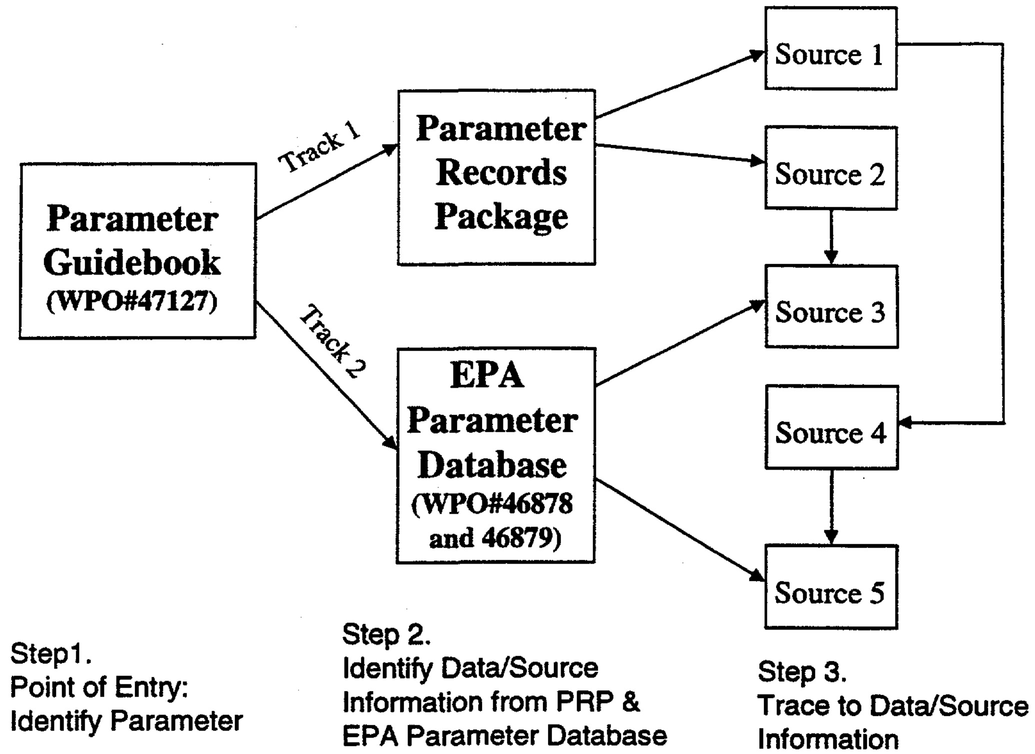


Figure 13. WIPP CCA PA Parameter tracking process.

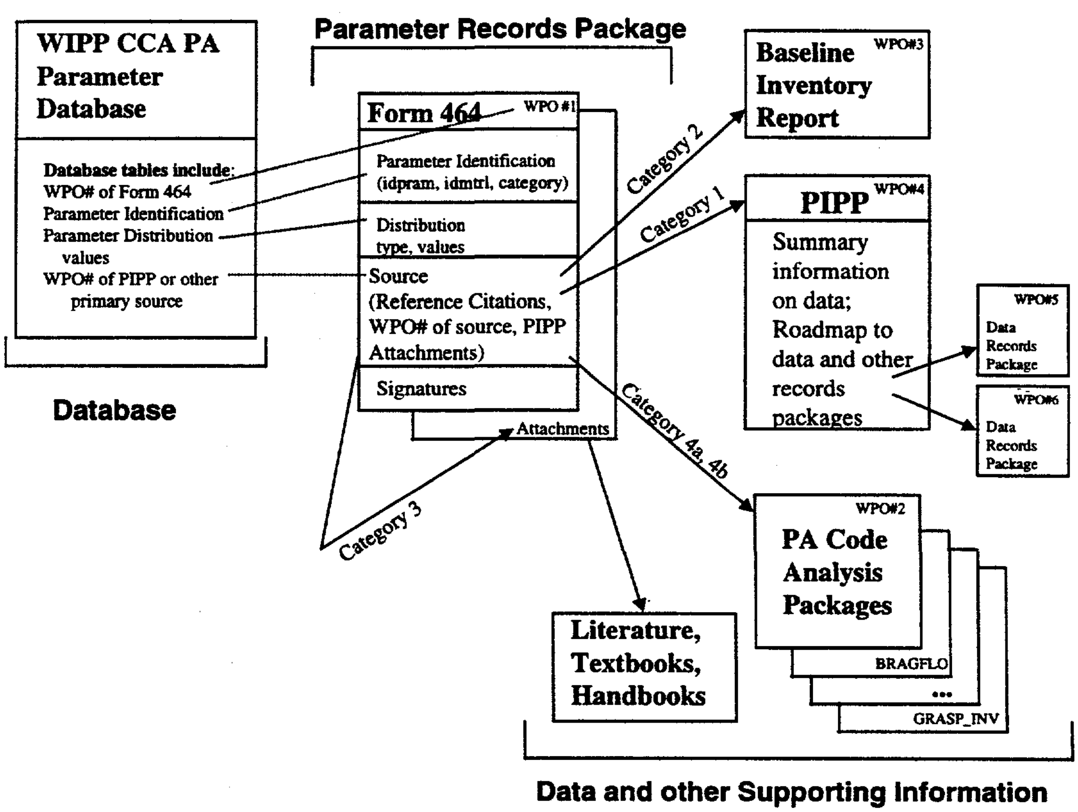


Figure 14. Parameter Records Package tracking system.

For some parameters, the PRP also includes additional supporting information attached to Form 464 (e.g., information generated by the PTL and/or information included for clarification) or information referenced on Form 464 by WPO number or with a document citation.

With the PRP in hand, users can track to the supporting information from Form 464, which is contained in the PRP. (In some cases, Form 464 is the PRP.) The type of supporting information available for a particular parameter is largely dependent on the category assigned to the parameter, as shown in Figure 14. Tracing to the supporting documentation for a particular parameter requires information found in the "Source" block or attached to Form 464. Supplementary information may be found in memoranda or other documentation included in or referenced within the PRP.

Category 1 parameters, those based on empirical data, are the most difficult to trace because of the sheer volume of data, supporting information, and documentation. Category 1 parameters are typically supported by PIPPs (see Section 4.2.2.) and Technical and Data Records Packages, which contain laboratory, field, and/or technical literature or data. The WPO number for the PIPP is found in the "Source" block of Form 464. A roadmap that contains pointers to supporting technical and data records packages or source information (i.e., the WPO number or other reference citation) is found in the PIPP. Additional links to supporting information are provided in the EPA Parameter Database (see Section 7.2). The PIPPs, which are identified by WPO number on Form 464, were created to link the Data Records Packages and/or other supporting information to the parameter distributions found in the PRPs. The PIPPs provide consistent, traceable links (in summary format) between PA database parameters and data packages, provide data summaries, identify related interpretive codes and references (including reports and test plans), and, where applicable, provide a summary of experimental data collection.

In some cases a single PIPP supports a single parameter; in other cases a single PIPP may support multiple parameters; in still other cases a single parameter is supported by multiple PIPPs (e.g., if a parameter was developed by combining laboratory and field data and separate PIPPs were assembled for the two data sets).

For Category 1 and 4a parameters, it is important to move down from the PRP through the PIPP to the data records and technical packages. If users enter the process in the middle—for example, by starting with the PIPP instead of the PRP—important information may be missed; that is, the user might miss reading a memorandum contained in the PRP that describes certain new information that supersedes the information contained in the PIPP. Likewise, by starting with a technical data package instead of the PRP, a user might miss information in the PRP or PIPP that points to documentation explaining that certain data were not qualified and are therefore unusable.

For Category 2 and 3 parameters, supporting documentation or references to supporting documentation (i.e., WPO numbers of documents available from the SWCF or citations) are either identified in the "Source" block of Form 464 or contained within the PRP. Supplementary information is included in the EPA Parameter Database.

Category 2 parameters are primarily supported by information found in the WIPP BIR. Pointers (i.e., the WPO number or other reference citation) to supporting documents are found in the "Source" section of the Form 464. Additional links to supporting information are provided in the EPA Parameter Database (see Section 7.2).

Category 3 parameters are supported by technical literature, handbooks, and textbooks. Pointers (i.e., the WPO number or other reference citation) to supporting documents are found in the "Source" block of Form 464. In addition, a copy of the page or pages from the source document and any minor calculations are attached to Form 464 and comprise the PRP. Additional links to supporting information are provided in the EPA Parameter Database (see Section 7.2).

Category 4a parameters are analogues, and supporting information may be linked back to Category 1 parameters or other supporting information. Supporting information for Category 4a parameters is found primarily in the PA Code Analysis Packages (see Sections 4.2.5 through 4.2.7.). Because the PA Code Analysis Packages were not complete at the time the Form 464s were completed and used, there is no direct link to these analysis packages on Form 464. However, links are provided in memoranda referenced in or attached to Form 464 and the PRP. Additional links to supporting information are provided in the EPA Parameter Database (see Section 7.2).

Category 4b parameters, including model configuration and legacy and placeholder parameters, are linked directly to the supporting information via Form 464 or indirectly to the PA Code Analysis Packages. Because the PA Code Analysis Packages were not complete at the time the Form 464s were completed and used, there is no direct link to the Category 4a parameter packages on Form 464. However, links are provided in memoranda referenced in or attached to Form 464 and the PRP. Additional links to supporting information are provided in the EPA Parameter Database (see Section 7.2).

## 7.2 Track 2: Parameter Trace Using the EPA Parameter Database

As a result of parameter reviews by the EPA staff, as well as internal and external QA auditors, SNL technical staff, and others, additional or links to supporting documentation and/or clarification for many parameters was requested. The new links to source information and clarifications were documented in memoranda and filed within the appropriate PRP, attached to Form 464, included in the PRP or Form 464 correspondence files, and, in some cases, entered into the CCA PA Parameter Database. As this process continued, tracing through the additional supporting information to pertinent information became more and more cumbersome as the complexity of the information-linking network increased. In addition, no single source compiled all the information related to parameter development, documentation, and qualification.

As a result of the initial post-CCA submittal parameter and computer code review, SNL constructed a database to support the ongoing review efforts and centralize information related to the parameters. Specifically, this database was designed to:

1. provide more direct pathways to pertinent information supporting the justification and rationale for parameter distributions as used in the CCA calculations,
2. provide quick-look information related to the qualification of data supporting each parameter, and
3. provide a centralized location for the information related to CCA calculation parameters, including those for which the database units changed, parameters that were computed from database values, parameters for which the PAA superseded the database value with another value, and parameters that were not contained in the CCA PA Parameter Database.

To accommodate post-CCA submittal reviews, SNL assembled the *wipp_reference* database, referred to here as the EPA Parameter Database.

This section contains information about the contents of the EPA Parameter Database and a discussion of the use of this database as a second parameter traceability tool. Note that in order to thoroughly trace the development, documentation, and qualification of a parameter, the EPA Parameter Database should be used in conjunction with PRP traceability methods discussed in Section 7.1.

### 7.2.1 EPA Parameter Database Contents

Sandia assembled the EPA Parameter Database to meet three objectives. The database provides:

1. quick-look information related to the qualification of data supporting each parameter;
2. a centralized location for the information related to CCA calculation parameters, including those for which the database units changed, those that were computed from database values, those for which the PAA superseded the database value with another value, and those that were not contained in the CCA PA Parameter Database;
3. a more direct pathway to pertinent information supporting the justification and rationale for parameter distributions as used in the CCA calculations.

Much of the information contained in the EPA Parameter Database is found in the CCA PA Parameter Database; however, additional information included in the EPA Parameter Database is not found in the CCA PA Parameter Database.

The EPA Parameter Database contains a table (provided in Appendix M1) entitled "CCA Parameter Listing"; this table addresses the questions regarding objectives 1 and 2 above. Five field column headings contain the following specific questions:

1. Is the parameter in the CCA database (Y/N)?
2. If the values used in the CCA are not the same as in the CCA database, provide the % difference.
3. Is the 464 consistent with the parameter in DB [CCA database] (Y/N/NA)?
4. Were the data developed under an NQA-1 Program?
5. Which methods were used to qualify existing data?

Appendix M6 contains memoranda that describe in detail each of the fields in the EPA Parameter Database tables including these five questions. Appendix N contains listings of parameters used in the CCA calculations for which the values differed from those listed in the database.

In response to the third objective, SNL created two other tables in the EPA Parameter Database that provide a more direct pathway to pertinent information supporting the justification and rationale for parameter distributions as used in the CCA calculations. These tables are included in Appendices M2 and M3. The table included in Appendix M2 is entitled "Additional Sources" and contains "Technical Traceability Documentation" fields. The table included as Appendix M3 is entitled "Enhanced Sources" and contains "Enhanced Source or Other Additional Information" fields.

For completeness, Appendix M4 contains a table from the EPA Parameter Database that provides a cross-reference to sources. This table includes information such as the reference identifier, title, journal, author, editor, date, publisher, and location. Appendix M5 contains a cross-reference linking each parameter with the code that used it in the CCA calculations. Appendix M6 contains a memorandum that describes the fields in the EPA Parameter Database tables. Table 16 lists the contents of the EPA Parameter Database.

Table 16. Contents of EPA Parameter Database Tables

| Table Name | Table Description and Contents |
|---|---|
| desc_1300 and nondb_parameters*<br><br>**all nondb_nnnn tables contain information about parameters used in the CCA calculation but not stored in the database.* | Contains the parameter information normally associated with a majority of the parameters.<br>id - A unique identifier assigned to a unique combination of material and property which define a parameter.<br>idmtrl - An 8-character (maximum) representation of a material.<br>idpram - An 8-character (maximum) representation of a property.<br>units - The units associated with the parameter.<br>distyp - The distribution type associated with a parameter.<br>mean - The mean value of the parameter.<br>median - The median value of the parameter.<br>stdev - The standard value of the parameter.<br>lowrange - The low range of the parameter.<br>hirange - The high range of the parameter.<br>active - A flag denoting whether or not the parameter is active.<br>impt - The category assigned to the parameter.<br>cataloger - The person who entered/updated/deactivated the parameter.<br>entrydate - The date the parameter's values were entered or updated or the date the parameter was deactivated.<br>class - Not used.<br>source - Not required. It was a shorthand way of determining who requested the parameter (PIxx or PAxx).<br>qualified - No longer used due to an ICN in QAP 9-2 and 9-4. |
| values_0800 | Contains the values of distributed values which cannot be accurately described via a maximum and minimum only.<br>id - Used to join the parameter to its distributed values.<br>pramval - The values to which a parameter can be distributed over when it cannot be accurately described by its low range and high range alone.<br>probability - The probability assigned to a distributed value.<br>idx - A numbering of the distributed values. |
| materials_0000 and nondb_mat_desc* | Contains a full description of the material denoted by the idmtrl.<br>id - Used to join the parameter to its material description.<br>mtrl_desc - A description of the material. |
| parameters_0000 and nondb_pram_desc* | Contains a full description of the property denoted by the idpram.<br>id - Used to join the parameter to its property description.<br>pram_desc - A description of the property. |

Table 16. Contents of EPA Parameter Database Tables

| Table Name | Table Description and Contents |
|---|---|
| model_0000 and nondb_model* | Contains the name of the code/model for which the parameter is required.<br>id - Used to join the parameter to the name of the code(s) it is utilized by.<br>codename - The name of the code(s) for which the parameter is required. |
| docu_0000 and nondb_docu* | Contains a reference id which relates a parameter to its source.<br>id - Used to join the parameter to its reference(s) or source(s).<br>refid - A 30-character representation of a unique source.<br>pagenum - The page number of the citation. |
| biblio_0000 | Contains a full citation of the source from which the parameter is based.<br>refid - Used to join the reference representation to its full citation.<br>title - The citation's title.<br>journal - If required, the name of the journal where the citation is found.<br>author - The author(s) of the citation.<br>editor - If available, the editor(s) of the citation.<br>date - The date the citation was published.<br>publisher - The publisher of the citation.<br>location - The location where the citation was published. |
| db_entry | Provides the information as to whether or not the parameter stored in the database was utilized by the codes, as stored.<br>id - Used to join the parameter to this table.<br>db_entry - Is the Parameter in the database (Y/N)?<br>percent_diff - If the values used in the CCA are not the same as in the database, provide the percent difference.<br>code_name - The name of the code(s) where the value used is different.<br>notes - Not used. |
| epa_info | Contains additional information for reviewers.<br>id - Used to join the parameter to this table.<br>Wpo_no - The WPO number assigned to a parameter.<br>consistent - Is the Form 464 consistent with the parameter in the database?<br>prof_judg - Classification of Data Category (footnote 2).<br>prof_adq - Not used. (Was professional judgment development adequate?)<br>nqa_dev - Were the data developed under an NQA-1 Program (Y/N)?<br>method - Which methods were used to qualify existing data? (footnote 3)<br>traceability - Not used. (Is there traceability from the parameter to the database?) |
| epa_add_info | Contains additional information concerning traceability for some parameters.<br>id - Used to join the parameter to this table.<br>ttd1 - Technical Traceability Documentation, first column.<br>ttd2 - Technical Traceability Documentation, second column.<br>ttd3 - Technical Traceability Documentation, third column.<br>ttd4 - Technical Traceability Documentation, fourth column.<br>enhanced1 - Enhanced Source or Other Additional Information, column 1<br>enhanced2 - Enhanced Source or Other Additional Information, column 2<br>enhanced3 - Enhanced Source or Other Additional Information, column 3 |

### 7.2.2 Tracing and Retrieving Parameter Information Using the EPA Parameter Database

This section contains information about the contents of the EPA Parameter Database tables, which provide more direct pathways to pertinent information supporting the justification and rationale for parameter distributions as used in the CCA calculations. These tables are included in Appendices M2 and M3.

In order to thoroughly trace the development, documentation, and qualification of a parameter, the EPA Parameter Database information should be used in conjunction with PRP traceability methods.

The reader must know the two-part name, id number, or the WPO number of the PRP for a parameter to be traced. Section 2 contains a full discussion of parameter identification.

As described, once the parameter id number or two-part name is known, users can enter the EPA Parameter Database (or use the tables and memoranda included in Appendices M1 through M6) and directly obtain the following:

1. quick-look information related to the qualification of data supporting each parameter;
2. information related to CCA calculation parameters, including those for which the database units changed, those that were computed from database values, those for which the PAA superseded the database value with another value, and those that were not contained in the CCA PA Parameter Database;
3. a more direct pathway to pertinent information supporting the justification and rationale for parameter distributions as used in the CCA calculations.

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