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**TECHNICAL SUPPORT DOCUMENT FOR SECTION 194.23**

**REVIEW OF CHANGES TO THE WIPP  
PERFORMANCE ASSESSMENT  
PARAMETERS SINCE THE 2004 PABC**

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## TABLE OF CONTENTS

1.0	Introduction.....	1
2.0	Approach.....	2
3.0	Review of Parameters used in CRA-2009 that have Changed Since PABC-2004.....	4
3.1	Parameter Value Review for CRA-2009 .....	19
3.1.1	New Parameters .....	19
3.1.2	Changed Parameters.....	20
3.2	Review of PAPDB Database-to-Code Interface for CRA-2009.....	22
3.3	PA Code Input File Review for CRA-2009 .....	28
3.3.1	BRAGFLO Assessment .....	29
3.3.2	BRAGFLO_DBR Assessment.....	35
3.3.3	CUTTINGS_S Assessment.....	39
3.3.4	NUTS Assessment .....	40
3.3.5	CCDFGF Assessment .....	41
3.3.6	PRELHS Assessment.....	42
3.3.7	Summary of CRA-2009 Input File Review .....	42
3.3.8	Summary of EPA CRA-2009 Completeness Issues Related to Parameters.....	43
4.0	Review of Parameters used in PABC-2009 that have Changed since CRA-2009 .....	47
4.1	Parameter Value Review for PABC-2009 .....	66
4.1.1	New Parameters .....	66
4.1.2	Changed Parameters.....	67
4.2	Review of PAPDB Database-to-Code Interface for PABC-2009.....	71
4.3	PA Code Input File Review for PABC-2009.....	81
4.3.1	BRAGFLO Assessment .....	82
4.3.2	BRAGFLO_DBR Assessment.....	84
4.3.3	CUTTINGS_S Assessment.....	88
4.3.4	NUTS Assessment .....	88
4.3.5	PANEL Assessment.....	90
4.3.6	MODFLOW Assessment .....	91
4.3.7	SECOTP2D Assessment.....	92
4.3.8	EPAUNI Assessment .....	94
4.3.9	CCDFGF Assessment .....	95
4.3.10	PRELHS Assessment.....	95
4.3.11	Summary of PABC-2009 Input File Review .....	96
5.0	Status of Prior EPA Recommendations for Hand-Coded Parameters .....	97
6.0	Parameter Data Entry Process Review .....	101
7.0	Review of Computing Hardware .....	102
8.0	Conclusions.....	103
	References.....	104

## LIST OF TABLES

Table 1.	Parameters Used in CRA-2009 that have Changed since PABC-2004 .....	5
Table 2.	Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004.....	9
Table 3.	Database-Code Interface Test Results for Parameters Used in CRA-2009 that have Changed since PABC-2004.....	23
Table 4.	CRA-2009 Hard Coded Inputs Recommended for Incorporation in the PAPDB .....	44
Table 5.	Summary of EPA CRA-2009 Completeness Issues Related to Parameters .....	46
Table 6.	Parameters Used in PABC-2009 that have Changed since CRA-2009 .....	48
Table 7.	Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009.....	53
Table 8.	Database-Code Interface Test Results for Parameters Used in PABC-2009 that have Changed since CRA-2009 .....	73
Table 9.	Status of Prior EPA Recommendations for Hard-Coded Parameters.....	98

## ABBREVIATIONS AND ACRONYMS

CCA	Compliance Certification Application
CCDF	Complementary Cumulative Distribution Function
CFR	<i>Code of Federal Regulations</i>
CH	Contact-Handled
CPR	Cellulose, Plastic, and Rubber
CRA-2009	2009 Compliance Recertification Application
DBR	Direct Brine Release
DOE or the Department	U.S. Department of Energy
EPA or the Agency	U.S. Environmental Protection Agency
ERMS	Electronic Record Management System
FTP	File Transfer Protocol
GWB	Generic Weep Brine
HP	Hewlett Packard
PA	Performance Assessment
PABC-2009	2009 WIPP Performance Assessment Baseline Calculation
PAPDB	Performance Assessment Parameter Database
PDE	Parameter Data Entry
QA	Quality Assurance
RH	Remote-Handled
SAN	Storage Area Network
SNL	Sandia National Laboratories
TSD	Technical Support Document
WIPP	Waste Isolation Pilot Plant

## EXECUTIVE SUMMARY

This Technical Support Document (TSD) documents a review of changes to the Waste Isolation Pilot Plant (WIPP) performance assessment parameter database for the 2009 WIPP Performance Assessment Baseline Calculation (PABC-2009). This is the fourth in a series of parameter reviews conducted by the U.S. Environmental Protection Agency (the Agency or EPA) since the original WIPP certification. The first three reviews evaluated development of the Performance Assessment Parameter Database (PAPDB) using a new computing platform and software, as well as changes made to the PAPDB for the U.S. Department of Energy's first Compliance Recertification Application in 2004 (CRA-2004). This fourth review evaluated the procedural and technical adequacy of changes made to the 2004 database for the Department's second Compliance Recertification Application in 2009.

No significant database problems were identified in this review. Of the approximately 1700 parameters in the PAPDB, 255 changes were made since 2004 that included 109 new parameters and 146 changes to the values of existing parameters. Most of the new parameters were introduced to either support new chemistry models or were replacements for parameters that were previously hand-coded (manually input) into the input files for the performance assessment codes. The Agency has recommended transferring parameters to the PAPDB because of the enhanced traceability that the database provides. Changes to the values of existing parameters occurred primarily because of an update to the waste inventory that prompted not only inventory changes but also changes in solubility and density data. Other changes occurred due to updated hydrogeologic analyses and updated Delaware Basin drilling and plugging practices. All parameter distributions, values, and units were correctly entered into the PAPDB and were technically adequate and appropriate.

A check of primary and secondary supporting documents was made for all parameter changes and all documents were quickly retrieved from the WIPP Records Center. All documentation was found to be complete and accurate, with the single exception of a misidentified table that will be corrected by DOE. The outcome of this check sufficiently supports the conclusion that the necessary documents are readily available to support the new and updated parameters. A database interface evaluation was performed for all new and changed parameters and the correct parameter values were retrieved from the PAPDB for each parameter. Changes to the performance assessment input file codes were reviewed for the presence of hand-coded parameter values that may have little or difficult traceability that would be better drawn from the PAPDB. Several parameters were moved into the PAPDB as a result of this review, and additional code comments were provided to enhance traceability for those hand-coded values used as numerical and run controls not appropriate to be drawn from the PAPDB.

Updated procedures for developing, documenting, controlling, and changing parameters, and for entering those parameters into the PAPDB, were also reviewed. The Agency found all procedural changes to be consistent with earlier versions and found all revisions to be appropriate.

## 1.0 INTRODUCTION

The ability of the U.S. Department of Energy (the Department or DOE) Waste Isolation Pilot Plant (WIPP) facility to continue to meet the certification requirements of the U.S. Environmental Protection Agency (the Agency or EPA) is demonstrated in part through the use of a series of performance assessment (PA) computer codes that are documented in the periodic DOE Compliance Recertification Applications (CRAs). This Technical Support Document describes the Agency's review of the Performance Assessment Parameter Database (PAPDB), parameter traceability, adequacy of parameter documentation, and changes to the performance assessment parameters used to support DOE's 2009 CRA. The results of this review document the Agency's evaluation of DOE's compliance with the requirements of 40 CFR 194.23(c)(4).

The PAPDB is a computerized database that contains the values of parameters used in PA calculations and is directly linked to the VMS operating system used for parameter retrieval for PA runs. The PAPDB also records a history of parameter value changes for different PA runs. It identifies metadata, such as parameter names, units, and distribution characteristics, and it identifies supporting documentation.

The previous recertification application was prepared by DOE in 2004. The Department's initial 2004 application, herein identified as CRA-2004, was reviewed by EPA and the CRA-2004 PA was modified at the Agency's request. The resubmitted PA, herein identified as the 2004 Performance Assessment Baseline Calculation (PABC-2004), was approved by the Agency and became the updated compliance baseline. Pursuant to the requirement to recertify the WIPP facility at 5-year intervals, DOE submitted a new compliance recertification application in March 2009, herein identified as CRA-2009. This application was reviewed by EPA and the PA was again modified at the Agency's request. The resubmitted PA is herein identified as the 2009 Performance Assessment Baseline Calculation (PABC-2009).

This parameter review was conducted in two stages, commensurate with the sequence of DOE recertification submittals. The first stage review evaluated changes in the parameter database between PABC-2004 and CRA-2009, and the second stage evaluated changes in the parameter database between CRA-2009 and PABC-2009.

## 2.0 APPROACH

This review was conducted by Agency and contractor personnel. The scope of the review included the following:

- Verification and documentation of changes to the PAPDB since PABC-2004
- Reviewing procedural documentation supporting database changes
- Reviewing and evaluating supporting metadata for new and changed parameter values
- Checking the ability of PA codes to accurately access input parameters from the new database
- Review of differences between the current and previous PA code input files on the VMS operating system to identify parameters not in the PAPDB

The primary objective of the Agency's review was to assess the transcription accuracy, documentation, and traceability of changes to the parameter values and metadata that have occurred in the PAPDB since PABC-2004. A secondary objective was to determine if all parameters used in the PA calculations were in the PAPDB.

Review of the parameter changes was initiated in May 2009 with preparatory activities and an on-site review of the PAPDB and its PA code interfaces. The PAPDB parameter database and associated metadata are maintained in Carlsbad, New Mexico, by DOE's WIPP science advisor, Sandia National Laboratories (SNL). Hard copies of documentation supporting the parameters and their values are maintained in SNL's WIPP Records Center in Carlsbad. The supporting documents are tracked by SNL's Electronic Record Management System (ERMS), through which a unique identifying number is assigned to each document.

The Agency's review of the two recertification applications was implemented in several steps, recognizing that changes in approach might be needed as the review progressed. Preparatory activities were conducted prior to the onsite reviews, included providing DOE with an advance list of review activities, obtaining a list of all parameters changed or added to the database since the previous PA, and scheduling review activities with SNL staff.

The first set of parameter changes, from PABC-2004 to CRA-2009, consisted of 90 new parameters and 16 changes in parameters since PABC-2004. The second set of parameter changes, from CRA-2009 to PABC-2009, consisted of 19 new parameters and 130 parameter value changes since CRA-2009. The following activities were conducted in reviewing parameter changes from PABC-2004 to CRA-2009 during the Agency review team's May 2009 visit to Carlsbad:

- Reviewed accuracy of data entry into the PAPDB by visually comparing the online PAPDB values with the values on the Parameter Data Entry (PDE) forms for every new and changed parameter. Parameter units, distribution type, statistics, names, and references also were reviewed.

- Checked PDE forms of all new and changed parameters for completeness, signatures, and references to supporting justification documentation.
- Reviewed supporting documentation identified on the PDE forms for every new and changed parameter to confirm accuracy of parameter values on the PDE forms and to evaluate the traceability of the parameter changes.
- Reviewed the ability of the current PA codes to accurately access every new and changed input parameter from the database.
- Reviewed the differences in input files between PABC-2004 and CRA-2009 for all input files that accessed parameter values in the CRA-2009 analysis to identify hand-coded parameters that should have been drawn from the PAPDB.

Follow-up activities were subsequently conducted by e-mail and telephone. SNL provided copies of documentation for parameters changed since PABC-2004 and copies of input file difference scripts for the input files that accessed parameter values in the CRA-2009 analysis. These documents were reviewed by the Agency review team to assess the appropriateness of the parameter changes and hand-coding practices. SNL also provided additional supporting documentation as requested to address issues that developed as the review of the database changes continued.

In February 2010, the Agency review team made a second visit to Carlsbad to review parameter changes between CRA-2009 and PABC-2009. The Agency team applied the same approach to this review as described above for the PABC-2004 to CRA-2009 review. In addition, the team reviewed applicable data entry and handling procedures, performed a comprehensive check of DOE's response to the Agency's previous recommendations for moving hand-coded parameters to the PAPDB, and reviewed documentation supporting the values of the parameters that had been moved to the PAPDB, as well as those that had not been moved.



### **3.0 REVIEW OF PARAMETERS USED IN CRA-2009 THAT HAVE CHANGED SINCE PABC-2004**

This review evaluated 90 new parameters and 16 changes to existing parameters out of the approximately 1,700 parameters currently in the PAPDB. The new and changed parameters are identified in Table 1. Table 1 presents the parameter names (consisting of a material name and a property name), the distribution type, the parameter value used in the CRA-2009 analysis, the previous parameter value, the parameter units, and the PA code(s) using the parameter. Parameter Data Entry (PDE) form provides the source information for parameter values and associated metadata to be entered into the PAPDB. The parameter values and metadata entered into the PAPDB were visually compared with those on the PDE forms and no discrepancies were identified.

Table 2 summarizes an assessment of the adequacy of supporting documentation for justifying the parameter changes. Table 2 provides the parameter name (material and property names), a description of the parameter type, ERMS numbers for the PDE form and supporting document, the effective date of the change, and comments that summarize the basis for the change.<sup>1</sup> In each case, the supporting document(s) provided adequate justification for the change. Also in each case, the supporting document(s) were consistent with the values and metadata in the PAPDB.

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<sup>1</sup> Parameter Data Entry (PDE) forms are identified by ERMS number in this report and are not included in the reference list.

**Table 1. Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Distribution Type	Parameter Value Used in CRA-2009				Previous Parameter Value				Parameter Units	Used in Code
			Mean	Median	Minimum	Maximum	Mean	Median	Minimum	Maximum		
BLOWOUT	MAXFLOW	Constant	3.888E+05	3.888E+05	3.888E+05	3.888E+05	9.504E+05	9.504E+05	9.504E+05	9.504E+05	seconds	BRAGFLO / DBR
BOREHOLE	TAUFAIL	Loguniform	10.5	1.96	0.05	77	Value was modified from PABC-2004 for AP-131 and changed back to its PABC-2004 value for CRA-2009				Pa	CUTTINGS_S / PRELHS
CAVITY_1	RELP_MOD	Constant	11	11	11	11	4	4	4	4	None	BRAGFLO
CAVITY_2	RELP_MOD	Constant	11	11	11	11	4	4	4	4	None	BRAGFLO
CAVITY_3	RELP_MOD	Constant	11	11	11	11	4	4	4	4	None	BRAGFLO
CAVITY_4	RELP_MOD	Constant	11	11	11	11	4	4	4	4	None	BRAGFLO
DRZ_0	POROSITY	Cumulative	2.11E-02	1.29E-02	3.90E-03	5.48E-02	1.565E-02	1.290E-02	3.900E-03	3.290E-02	None	BRAGFLO
DRZ_1	POROSITY	Cumulative	2.11E-02	1.29E-02	3.90E-03	5.48E-02	1.565E-02	1.290E-02	3.900E-03	3.290E-02	None	BRAGFLO / DBR
DRZ_PCS	POROSITY	Cumulative	2.11E-02	1.29E-02	3.90E-03	5.48E-02	1.565E-02	1.290E-02	3.900E-03	3.290E-02	None	BRAGFLO
EXP_AREA	RELP_MOD	Constant	11	11	11	11	4	4	4	4	None	BRAGFLO
GLOBAL	LAMBDAD	Constant	5.85E-03	5.85E-03	5.85E-03	5.85E-03	5.25E-03	5.25E-03	5.25E-03	5.25E-03	1/km <sup>2</sup> *yr	PRECCDFGF
OPS_AREA	RELP_MOD	Constant	11	11	11	11	4	4	4	4	None	BRAGFLO
REFCON	DN_CELL	Constant	1100	1100	1100	1100	New parameter				kg/m <sup>3</sup>	BRAGFLO / DBR
REFCON	DN_FE	Constant	7870	7870	7870	7870	New parameter				kg/m <sup>3</sup>	BRAGFLO / DBR
REFCON	DN_FEOH2	Constant	3400	3400	3400	3400	New parameter				kg/m <sup>3</sup>	BRAGFLO / DBR
REFCON	DN_FES	Constant	4700	4700	4700	4700	New parameter				kg/m <sup>3</sup>	BRAGFLO / DBR
REFCON	DN_MGCO3	Constant	3050	3050	3050	3050	New parameter				kg/m <sup>3</sup>	BRAGFLO / DBR
REFCON	DN_MGO	Constant	3600	3600	3600	3600	New parameter				kg/m <sup>3</sup>	BRAGFLO / DBR
REFCON	DN_MGOH2	Constant	2370	2370	2370	2370	New parameter				kg/m <sup>3</sup>	BRAGFLO / DBR
REFCON	DN_SALT	Constant	2180	2180	2180	2180	New parameter				kg/m <sup>3</sup>	BRAGFLO / DBR
REFCON	FVW	Constant	3.85E-01	3.85E-01	3.85E-01	3.85E-01	3.86E-01	3.86E-01	3.86E-01	3.86E-01	None	PRECCDFGF
REFCON	MW_FEOH2	Constant	8.9860E-02	8.9860E-02	8.9860E-02	8.9860E-02	New parameter				kg/mole	BRAGFLO
REFCON	MW_FES	Constant	8.7911E-02	8.7911E-02	8.7911E-02	8.7911E-02	New parameter				kg/mole	BRAGFLO
REFCON	MW_MGCO3	Constant	8.4314E-02	8.4314E-02	8.4314E-02	8.4314E-02	New parameter				kg/mole	BRAGFLO
REFCON	MW_MGO	Constant	4.0304E-02	4.0304E-02	4.0304E-02	4.0304E-02	New parameter				kg/mole	BRAGFLO
REFCON	MW_MGOH2	Constant	5.8320E-02	5.8320E-02	5.8320E-02	5.8320E-02	New parameter				kg/mole	BRAGFLO
REFCON	STCO_11	Constant	1	1	1	1	New parameter				None	BRAGFLO
REFCON	STCO_12	Constant	-2	-2	-2	-2	New parameter				None	BRAGFLO
REFCON	STCO_13	Constant	-1	-1	-1	-1	New parameter				None	BRAGFLO

**Table 1. Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Distribution Type	Parameter Value Used in CRA-2009				Previous Parameter Value				Parameter Units	Used in Code
			Mean	Median	Minimum	Maximum	Mean	Median	Minimum	Maximum		
REFCON	STCO_14	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_15	Constant	1	1	1	1	New parameter				None	BRAGFLO
REFCON	STCO_16	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_17	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_18	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_19	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_21	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_22	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_23	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_24	Constant	-1	-1	-1	-1	New parameter				None	BRAGFLO
REFCON	STCO_25	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_26	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_27	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_28	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_29	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_31	Constant	-1	-1	-1	-1	New parameter				None	BRAGFLO
REFCON	STCO_32	Constant	2	2	2	2	New parameter				None	BRAGFLO
REFCON	STCO_33	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_34	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_35	Constant	-1	-1	-1	-1	New parameter				None	BRAGFLO
REFCON	STCO_36	Constant	1	1	1	1	New parameter				None	BRAGFLO
REFCON	STCO_37	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_38	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_39	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_41	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_42	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_43	Constant	-1	-1	-1	-1	New parameter				None	BRAGFLO
REFCON	STCO_44	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_45	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_46	Constant	1	1	1	1	New parameter				None	BRAGFLO
REFCON	STCO_47	Constant	0	0	0	0	New parameter				None	BRAGFLO

**Table 1. Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Distribution Type	Parameter Value Used in CRA-2009				Previous Parameter Value				Parameter Units	Used in Code
			Mean	Median	Minimum	Maximum	Mean	Median	Minimum	Maximum		
REFCON	STCO_48	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_49	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_51	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_52	Constant	-1	-1	-1	-1	New parameter				None	BRAGFLO
REFCON	STCO_53	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_54	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_55	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_56	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_57	Constant	-1	-1	-1	-1	New parameter				None	BRAGFLO
REFCON	STCO_58	Constant	1	1	1	1	New parameter				None	BRAGFLO
REFCON	STCO_59	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_61	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_62	Constant	1	1	1	1	New parameter				None	BRAGFLO
REFCON	STCO_63	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_64	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_65	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_66	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_67	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_68	Constant	-1	-1	-1	-1	New parameter				None	BRAGFLO
REFCON	STCO_69	Constant	1	1	1	1	New parameter				None	BRAGFLO
REFCON	STCO_71	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_72	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_73	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_74	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_75	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_76	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_77	Constant	-1	-1	-1	-1	New parameter				None	BRAGFLO
REFCON	STCO_78	Constant	0	0	0	0	New parameter				None	BRAGFLO
REFCON	STCO_79	Constant	1	1	1	1	New parameter				None	BRAGFLO
REPOSIT	RELP_MOD	Constant	12	12	12	12	4	4	4	4	None	BRAGFLO

**Table 1. Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Distribution Type	Parameter Value Used in CRA-2009				Previous Parameter Value				Parameter Units	Used in Code
			Mean	Median	Minimum	Maximum	Mean	Median	Minimum	Maximum		
S_HALITE	POROSITY	Cumulative	1.82E-02	1.00E-02	1.00E-03	5.19E-02	1.28E-02	1.00E-02	1.00E-03	3.00E-02	None	BRAGFLO / DBR / PRELHS
WAS_AREA	BRUCITEC	Constant	0	0	0	0	New parameter				moles/kg*s	BRAGFLO
WAS_AREA	BRUCITEH	Constant	2.10E-09	2.10E-09	2.10E-09	2.10E-09	New parameter				moles/kg*s	BRAGFLO
WAS_AREA	BRUCITES	Constant	2.60E-08	2.60E-08	2.60E-08	2.60E-08	New parameter				moles/kg*s	BRAGFLO
WAS_AREA	MGO_EF	Constant	1.2	1.2	1.2	1.2	New parameter				None	BRAGFLO
WAS_AREA	DCELCCHW	Constant	0	0	0	0	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DCELCRHW	Constant	0	0	0	0	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DCELECHW	Constant	1.22	1.22	1.22	1.22	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DCELERHW	Constant	0	0	0	0	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DPLSECHW	Constant	8.76	8.76	8.76	8.76	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DPLSERHW	Constant	0	0	0	0	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DRUBCCHW	Constant	0	0	0	0	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DRUBCRHW	Constant	0	0	0	0	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DRUBECHW	Constant	0	0	0	0	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DRUBERHW	Constant	0	0	0	0	New parameter				kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	RELP_MOD	Constant	12	12	12	12	4	4	4	4	None	BRAGFLO / DBR

**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
BLOWOUT	MAXFLOW	Maximum duration of blowout flow for direct brine releases	546059	545988	4/30/2007	The maximum duration of direct brine releases was changed from 11 days to 4.5 days, based on distinguishing between blowouts from brine-producing zones and blowouts from gas-producing zones, which can have longer durations if a gas fire occurs. The previous maximum duration was based on a 1978 worst-case gas well blowout and fire. The revised value of 4.5 days is based on updated interviews with area drillers and mud engineers, assuming a maximum repository brine pressure equal to the lithostatic pressure of 14.9 MPa, and including contingencies for possible delays. EPA reviewed the basis for reducing the maximum brine release duration and found it to be adequately justified.
BOREHOLE	TAUFAIL	Effective shear strength for erosion of borehole and fill	547524	547515	12/7/2007	The lower limit of this parameter was changed from its PABC-2004 value for the intermediate analysis AP-131, and then changed back to its PABC-2004 value for the CRA-2009 analysis. As a result, the CRA-2009 cavings releases are identical to the PABC-2004 releases. EPA finds this to be acceptable.
CAVITY_1	RELP_MOD	Relative permeability model for waste area	545790	545764	4/11/2007	This parameter implements a new model for the capillary pressure and relative permeability of open cavities. This new model removes capillary pressure effects from the calculation of relative permeability. The supporting document was reviewed by EPA and the model change was found to be justified.
CAVITY_2	RELP_MOD	Relative permeability model for non-waste area	545791	545764	4/11/2007	Same comment as for CAVITY_1:RELP_MOD.
CAVITY_3	RELP_MOD	Relative permeability model for shaft	545792	545764	4/11/2007	Same comment as for CAVITY_1:RELP_MOD.
CAVITY_4	RELP_MOD	Relative permeability model for borehole	545793	545764	4/11/2007	Same comment as for CAVITY_1:RELP_MOD.
DRZ_0	POROSITY	Effective DRZ porosity for time period minus 5 to 0 years	545794	545755	4/10/2007	The identification number of the associated analysis plan was manually corrected on the PDE form and initialed by the PDE requester; this change is therefore acceptable. These parameter value changes correct the previous porosity based on weight percent to a porosity based on volume fraction. Following current WIPP PA practice, these parameter values were determined by increasing S_HALITE:POROSITY values by 0.0029. The supporting document was reviewed by EPA and these parameter changes were found to be justified. However, EPA found that the supporting document recommended applying this change to DRZ_2:POROSITY as well as to DRZ_0:POROSITY and DRZ_1:POROSITY. The parameter DRZ_2:POROSITY was not among those changed by DOE for the CRA-2009 analysis. DRZ_2:POROSITY was not listed as a changed parameter because it was created for a postponed 2007 peer review and is not used in compliance calculations.
DRZ_1	POROSITY	Effective DRZ porosity for time period 0 to complete healing	545795	545755	4/10/2007	Same comment as for DRZ_0:POROSITY.

**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
DRZ_PCS	POROSITY	Effective DRZ porosity above concrete portion of panel closure	547522	547486	12/6/2007	The above changes in the porosity distributions for materials DRZ_0 and DRZ_1 inadvertently omitted changes in the porosity distribution for material DRZ_PCS. This change makes the distribution of DRZ_PCS:POROSITY the same as the distributions for DRZ_0:POROSITY and DRZ_1:POROSITY. EPA found this change to be justified.
EXP_AREA	RELP_MOD	Relative permeability model for experimental area	545802	545764	4/11/2007	Same comment as for CAVITY_1:RELP_MOD.
GLOBAL	LAMBDA	Drilling rate per unit area	547523	547515	12/7/2007	The change in this parameter value represents the increase in drilling rates in the Delaware Basin since the PABC-2004, as determined in a 2007 DOE survey. EPA found this change to be justified.
OPS_AREA	RELP_MOD	Relative permeability model for operations area	545803	545764	4/11/2007	Same comment as for CAVITY_1:RELP_MOD.
REFCON	DN_CELL	Density of cellulose	545664	545611	3/19/2007	This is a new parameter required by BRAGFLO Version 6.0 to calculate the volume of chemical constituents produced or consumed by certain chemical reactions. The value of this parameter was set equal to the density of cellulose determined in a previous WIPP analysis and recorded on page 17 of the SNL Report SAND97-0796. EPA checked the value against that source and it was found to be accurately transcribed.
REFCON	DN_FE	Density of Fe	545664	545611	3/19/2007	This is a new parameter required by BRAGFLO Version 6.0 to calculate the volume of chemical constituents produced or consumed by certain chemical reactions. The density value was taken from a recognized standard source—the CRC Handbook of Chemistry and Physics, 78th Edition. EPA checked the value against that source and it was found to be accurately transcribed.
REFCON	DN_FEOH2	Density of FeOH2	545664	545611	3/19/2007	Same comment as for REFCON:DN_FE.
REFCON	DN_FES	Density of FeS	545664	545611	3/19/2007	Same comment as for REFCON:DN_FE.
REFCON	DN_MGCO3	Density of MgCO3	545664	545611	3/19/2007	Same comment as for REFCON:DN_FE.
REFCON	DN_MGO	Density of MgO	545664	545611	3/19/2007	Same comment as for REFCON:DN_FE.
REFCON	DN_MGOH2	Density of MgOH2	545664	545611	3/19/2007	Same comment as for REFCON:DN_FE.
REFCON	DN_SALT	Density of salt	545664	545611	3/19/2007	This parameter, the density of salt, is used in BRAGFLO and was given the same value as SPALLMOD:SALTDEN, which is used in DRSPALL as the density of solid cuttings from the Salado. EPA checked the value of this parameter against the value of SPALLMOD:SALTDEN and it was found to be accurately transcribed.

**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
REFCON	FVW	Fraction of repository volume occupied by waste	545666	545481 523760	3/13/2007	This parameter, the fraction of repository volume occupied by waste, is calculated by dividing REPOSIT:VOLCHW by REFCON:VREPOS. The value of REFCON:FVW was changed twice since the CCA. The value of REFCON:VREPOS was increased in 2002 to account for the volume of three exhaust and intake drifts that were inadvertently excluded from the original calculation. This correction is documented in Stein 2002 [ERMS 523760] and resulted in changing the rounded value of REFCON:FVW from 0.388 to 0.386. A rounding error was subsequently found that changed the revised value of REFCON:FVW from 0.386 to 0.385. This correction is documented in Kirchner 2007 [ERMS 545481]. SNL concluded and EPA concurs that the impact of using the value of 0.386 in PABC-2004 instead of 0.385 is not significant, particularly since it resulted in slightly overestimating the cuttings and spillings releases.
REFCON	MW_FEOH2	Molecular weight of FeOH2	545663	545611	3/19/2007	This is a new parameter required by BRAGFLO Version 6.0 to calculate the volume of chemical constituents produced or consumed by certain chemical reactions. The molecular weight was taken from a recognized standard source—the CRC Handbook of Chemistry and Physics, 78th Edition. EPA checked the value against that source and it was found to be accurately transcribed.
REFCON	MW_FES	Molecular weight of FeS	545663	545611	3/19/2007	Same comment as for REFCON:MW_FEOH2.
REFCON	MW_MGCO3	Molecular weight of MgCO3	545663	545611	3/19/2007	Same comment as for REFCON:MW_FEOH2.
REFCON	MW_MGO	Molecular weight of MgO	545663	545611	3/19/2007	Same comment as for REFCON:MW_FEOH2.
REFCON	MW_MGOH2	Molecular weight of MgOH2	545663	545611	3/19/2007	Same comment as for REFCON:MW_FEOH2.
REFCON	STCO_11	Fe corrosion:H2 stoichiometric coefficient	545660	545611	3/19/2007	The stoichiometric coefficients for the chemical reactions modeled in BRAGFLO Version 6.0 have been organized into a single matrix S(I,J), where I represents the reaction and J represents the individual species. A positive value of S(I,J) represents production and a negative value represents consumption. A zero value generally means that the species is not relevant to the reaction being modeled. For example, the species MgO is not relevant to the anoxic corrosion of iron. EPA checked the value of this coefficient against the chemical equation for anoxic iron corrosion and found it to be accurate.
REFCON	STCO_12	Fe corrosion:H2O stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_11.
REFCON	STCO_13	Fe corrosion:Fe stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_11.
REFCON	STCO_14	Fe corrosion:cellulosics stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_11.
REFCON	STCO_15	Fe corrosion:FeOH2 stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_11.



**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
REFCON	STCO_16	Fe corrosion:FeS stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_11.
REFCON	STCO_17	Fe corrosion:MgO stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_11.
REFCON	STCO_18	Fe corrosion:MgOH2 stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_11.
REFCON	STCO_19	Fe corrosion:MgCO3 stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_11.
REFCON	STCO_21	Microbial gas generation:H2 stoichiometric coefficient	545660	545611	3/19/2007	The stoichiometric coefficients for the chemical reactions modeled in BRAGFLO Version 6.0 have been organized into a single matrix S(I,J), where I represents the reaction and J represents the individual species. A positive value of S(I,J) represents production and a negative value represents consumption. A zero value generally means that the species is not relevant to the reaction being modeled. DOE used an average stoichiometric model for microbial gas generation, where the chemical reactions for consumption of organic carbon by denitrification and sulfate reduction reactions are replaced by a simplified chemical equation. EPA found that the value of this coefficient in the P/APDB is consistent with the assumptions of the average stoichiometric model and with the treatment of microbial gas generation in PA.
REFCON	STCO_22	Microbial gas generation: H2O stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_21.
REFCON	STCO_23	Microbial gas generation:Fe stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_21.
REFCON	STCO_24	Microbial gas generation: cellulose stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_21.
REFCON	STCO_25	Microbial gas generation: FeOH2 stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_21.
REFCON	STCO_26	Microbial gas generation:FeS stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_21.

**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
REFCON	STCO_27	Microbial gas generation: MgO stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_21.
REFCON	STCO_28	Microbial gas generation: MgOH2 stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_21.
REFCON	STCO_29	Microbial gas generation: MgCO3 stoichiometric coefficient	545660	545611	3/19/2007	Same comment as for REFCON:STCO_21.
REFCON	STCO_31	FeOH2 sulfidation:H2 stoichiometric coefficient	545661	545611	3/19/2007	The stoichiometric coefficients for the chemical reactions modeled in BRAGFLO Version 6.0 have been organized into a single matrix S(I,J), where I represents the reaction and J represents the individual species. A positive value of S(I,J) represents production and a negative value represents consumption. A zero value generally means that the species is not relevant to the reaction being modeled. For example, the species MgO is not relevant to iron hydroxide sulfidation. EPA checked the value of this coefficient against the chemical equation for iron hydroxide sulfidation and found it to be accurate.
REFCON	STCO_32	FeOH2 sulfidation:H2O stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_31.
REFCON	STCO_33	FeOH2 sulfidation:Fe stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_31.
REFCON	STCO_34	FeOH2 sulfidation:cellulosics stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_31.
REFCON	STCO_35	FeOH2 sulfidation:FeOH2 stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_31.
REFCON	STCO_36	FeOH2 sulfidation:FeS stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_31.
REFCON	STCO_37	FeOH2 sulfidation:MgO stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_31.
REFCON	STCO_38	FeOH2 sulfidation:MgOH2 stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_31.
REFCON	STCO_39	FeOH2 sulfidation:MgCO3 stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_31.

**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
REFCON	STCO_41	Metallic Fe sulfidation:H2 stoichiometric coefficient	545661	545611	3/19/2007	The stoichiometric coefficients for the chemical reactions modeled in BRAGFLO Version 6.0 have been organized into a single matrix S(I,J), where I represents the reaction and J represents the individual species. A positive value of S(I,J) represents production and a negative value represents consumption. A zero value generally means that the species is not relevant to the reaction being modeled. For example, the species MgO is not relevant to metallic iron sulfidation. However, in this chemical equation, H <sub>2</sub> S gas is converted to H <sub>2</sub> gas with no production or consumption of gas, and the stoichiometric coefficient for REFCON:STCO_41 is appropriately set to zero. EPA checked the value of this coefficient against the chemical equation for metallic iron sulfidation and found it to be accurate.
REFCON	STCO_42	Metallic Fe sulfidation:H2O stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_41.
REFCON	STCO_43	Metallic Fe sulfidation Fe stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_41.
REFCON	STCO_44	Metallic Fe sulfidation: cellulose stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_41.
REFCON	STCO_45	Metallic Fe sulfidation: FeOH2 stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_41.
REFCON	STCO_46	Metallic Fe sulfidation:FeS stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_41.
REFCON	STCO_47	Metallic Fe sulfidation:MgO stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_41.
REFCON	STCO_48	Metallic Fe sulfidation: MgOH2 stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_41.
REFCON	STCO_49	Metallic Fe sulfidation: MgCO3 stoichiometric coefficient	545661	545611	3/19/2007	Same comment as for REFCON:STCO_41.
REFCON	STCO_51	MgO hydration:H2 stoichiometric coefficient	545662	545611	3/19/2007	The stoichiometric coefficients for the chemical reactions modeled in BRAGFLO Version 6.0 have been organized into a single matrix S(I,J), where I represents the reaction and J represents the individual species. A positive value of S(I,J) represents production and a negative value represents consumption. A zero value generally means that the species is not relevant to the reaction being modeled. For example, the species Fe is not relevant to MgO hydration. EPA checked the value of this coefficient against the chemical equation for MgO hydration and found it to be accurate.
REFCON	STCO_52	MgO hydration:H2O stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_51.

**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
REFCON	STCO_53	MgO hydration:Fe stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_51.
REFCON	STCO_54	MgO hydration:cellulosics stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_51.
REFCON	STCO_55	MgO hydration:FeOH2 stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_51.
REFCON	STCO_56	MgO hydration:FeS stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_51.
REFCON	STCO_57	MgO hydration:MgO stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_51.
REFCON	STCO_58	MgO hydration:MgOH2 stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_51.
REFCON	STCO_59	MgO hydration:MgCO3 stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_51.
REFCON	STCO_61	MgOH2 carbonation:H2 stoichiometric coefficient	545662	545611	3/19/2007	The stoichiometric coefficients for the chemical reactions modeled in BRAGFLO Version 6.0 have been organized into a single matrix S(I,J), where I represents the reaction and J represents the individual species. A positive value of S(I,J) represents production and a negative value represents consumption. A zero value generally means that the species is not relevant to the reaction being modeled. For example, the species Fe is not relevant to magnesium hydroxide carbonation. EPA checked the value of this coefficient against the chemical equation for magnesium hydroxide carbonation and found it to be accurate.
REFCON	STCO_62	MgOH2 carbonation:H2O stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_61.
REFCON	STCO_63	MgOH2 carbonation:Fe stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_61.
REFCON	STCO_64	MgOH2 carbonation:cellulosics stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_61.
REFCON	STCO_65	MgOH2 carbonation:FeOH2 stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_61.
REFCON	STCO_66	MgOH2 carbonation:FeS stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_61.

**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
REFCON	STCO_67	MgOH2 carbonation:MgO stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_61.
REFCON	STCO_68	MgOH2 carbonation:MgOH2 stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_61.
REFCON	STCO_69	MgOH2 carbonation:MgCO3 stoichiometric coefficient	545662	545611	3/19/2007	Same comment as for REFCON:STCO_61.
REFCON	STCO_71	MgO carbonation:H2 stoichiometric coefficient	545663	545611	3/19/2007	The stoichiometric coefficients for the chemical reactions modeled in BRAGFLO Version 6.0 have been organized into a single matrix S(I,J), where I represents the reaction and J represents the individual species. A positive value of S(I,J) represents production and a negative value represents consumption. A zero value generally means that the species is not relevant to the reaction being modeled. For example, the species Fe is not relevant to MgO carbonation. EPA checked the value of this coefficient against the chemical equation for MgO carbonation and found it to be accurate.
REFCON	STCO_72	MgO carbonation:H2O stoichiometric coefficient	545663	545611	3/19/2007	Same comment as for REFCON:STCO_71.
REFCON	STCO_73	MgO carbonation:Fe stoichiometric coefficient	545663	545611	3/19/2007	Same comment as for REFCON:STCO_71.
REFCON	STCO_74	MgO carbonation:cellulosics stoichiometric coefficient	545663	545611	3/19/2007	Same comment as for REFCON:STCO_71.
REFCON	STCO_75	MgO carbonation:FeOH2 stoichiometric coefficient	545663	545611	3/19/2007	Same comment as for REFCON:STCO_71.
REFCON	STCO_76	MgO carbonation:FeS stoichiometric coefficient	545663	545611	3/19/2007	Same comment as for REFCON:STCO_71.
REFCON	STCO_77	MgO carbonation:MgO stoichiometric coefficient	545663	545611	3/19/2007	Same comment as for REFCON:STCO_71.
REFCON	STCO_78	MgO carbonation:MgOH2 stoichiometric coefficient	545663	545611	3/19/2007	Same comment as for REFCON:STCO_71.
REFCON	STCO_79	MgO carbonation:MgCO3 stoichiometric coefficient	545663	545611	3/19/2007	Same comment as for REFCON:STCO_71.
REPOSIT	RELP_MOD	Relative permeability model for regions outside panel	545800	545764	4/11/2007	This parameter implements a new model for the capillary pressure and relative permeability of waste-filled areas. This new model removes capillary pressure effects from the calculation of relative permeability. The supporting document was reviewed by EPA and the model change was found to be justified.

**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
S_HALITE	POROSITY	Effective porosity of intact Salado halite	545804	545755	4/10/2007	This parameter value change corrects the previous porosity based on weight percent to a porosity based on volume fraction. The supporting document was reviewed by EPA and this change was found to be justified.
WAS_AREA	BRUCITEC	MgO inundated hydration rate in ERDA-6 brine	545799	545757	4/11/2007	This is a new parameter required by BRAGFLO Version 6.0 to calculate the MgO hydration rate. The value of this parameter represents the experimentally determined hydration rate for inundated conditions with Castile brine from WIPP Well ERDA-6. The parameter value was conservatively set to zero pending completion of current experiments. EPA's review of the supporting document found the value of this parameter to be adequately justified.
WAS_AREA	BRUCITEH	MgO humid hydration rate	545799	545757	4/11/2007	This is a new parameter required by BRAGFLO Version 6.0 to calculate the MgO hydration rate. The value of this parameter represents the experimentally based hydration rate for humid conditions. Because the hydration rate was from a single experiment, a large subjective uncertainty was applied. EPA's review of the supporting document found this parameter to be adequately justified.
WAS_AREA	BRUCITES	MgO inundated hydration rate in GWB brine	545799	545757	4/11/2007	This is a new parameter required by BRAGFLO Version 6.0 to calculate the MgO hydration rate. The value of this parameter represents the experimentally determined hydration rate for inundated conditions with Generic Weep Brine (GWB), a synthetic brine representative of grain boundary fluids from the Salado. Because the hydration rate was from a single experiment, a large subjective uncertainty was applied. EPA's review of the supporting document found this parameter to be adequately justified.
WAS_AREA	MGO_EF	MgO excess factor: ratio of MgO to organic carbon in CPR	545665	545611	3/19/2007	This is a new parameter required by BRAGFLO Version 6.0 to calculate the volume of MgO placed in the repository. The value of this parameter represents the excess of moles of MgO over moles of organic carbon, and EPA considers a value of 1.2 to be appropriate.
WAS_AREA	DCELCCHW	Density of cellulose in CH waste container materials	545695	545689	3/30/2007	This is a new parameter required by BRAGFLO to calculate the effect of the organic carbon in waste containers and emplacement materials on repository gas production and the MgO excess factor. Only CHW emplacement materials contain significant quantities of cellulose and plastic. CHW emplacement materials contain little rubber and CHW container materials contain no cellulose, plastic, or rubber (CPR). RHW container and emplacement materials also contain no CPR. Materials with little or no CPR are assigned densities of zero. EPA found this assignment to be justified.
WAS_AREA	DCELCRHW	Density of cellulose in RH waste container materials	545695	545689	3/30/2007	Same comment as for WAS_AREA:DCELCCHW.
WAS_AREA	DCELECHW	Density of cellulose in CH waste emplacement materials	545695	545689	3/30/2007	This is a new parameter required by BRAGFLO to calculate the effect of the organic carbon in waste containers and emplacement materials on repository gas production and the MgO excess factor. The masses of cellulose and plastic in CHW emplacement materials were separately estimated by DOE. EPA found this assignment to be justified.
WAS_AREA	DCELERHW	Density of cellulose in RH waste emplacement materials	545695	545689	3/30/2007	Same comment as for WAS_AREA:DCELCCHW.

**Table 2. Justification Check for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
WAS_AREA	DPLSECHW	Density of plastics in CH waste emplacement materials	545695	545689	3/30/2007	Same comment as for WAS_AREA:DCELECHW.
WAS_AREA	DPLSERHW	Density of plastics in RH waste emplacement materials	545695	545689	3/30/2007	Same comment as for WAS_AREA:DCELCCHW.
WAS_AREA	DRUBCCHW	Density of rubber in CH waste container materials	545695	545689	3/30/2007	Same comment as for WAS_AREA:DCELCCHW.
WAS_AREA	DRUBCRHW	Density of rubber in RH waste container materials	545695	545689	3/30/2007	Same comment as for WAS_AREA:DCELCCHW.
WAS_AREA	DRUBECHW	Density of rubber in CH waste emplacement materials	545695	545689	3/30/2007	Same comment as for WAS_AREA:DCELCCHW.
WAS_AREA	DRUBERHW	Density of rubber in RH waste emplacement materials	545695	545689	3/30/2007	Same comment as for WAS_AREA:DCELCCHW.
WAS_AREA	RELP_MOD	Relative permeability model for waste and waste emplacement area	545801	545764	4/11/2007	Same comment as for REPOSIT:RELP_MOD.

### 3.1 PARAMETER VALUE REVIEW FOR CRA-2009

The results of EPA's parameter value review are summarized for new parameters in Section 3.1.1 and for existing parameters with changed values in Section 3.1.2.

#### 3.1.1 New Parameters

BRAGFLO Version 5.0 was used for PABC-2004. BRAGFLO Version 6.0 (Nemer 2007a [ERMS 545015]) was subsequently developed to incorporate additional capabilities and flexibility, and was used in CRA-2009. All of the new parameters required for CRA-2009 were needed because of the additional chemical capabilities in BRAGFLO Version 6.0. These additional capabilities included modeling MgO hydration reactions and adding additional flexibility in modeling CPR degradation, iron corrosion, iron sulfidation, and MgO carbonation reactions. This required the introduction of additional, constant value parameters used to describe the reactions and the chemical constituents. Although this additional capability now exists in BRAGFLO, only CPR degradation and corrosion of metallic iron were activated in CRA-2009. The MgO hydration reactions and the other degradation reactions are new to BRAGFLO and were deactivated in CRA-2009 by setting the relevant stoichiometric coefficients to zero in the PREBRAG input file (see PREBRAG input file review in Section 3.3.1). As implemented in CRA-2009, BRAGFLO Version 6.0, therefore, uses the same set of chemical reactions as previously used in BRAGFLO Version 5.0 for PABC-2004. None of the new parameters supporting the deactivated chemical reactions were therefore used in CRA-2009. A description of the additional chemistry parameters is presented in Clayton 2007c [ERMS 547515].

EPA has classified the new parameters into the following six groups:

*Group CRA-2009-N1* consists of the densities of cellulose, iron, and magnesium compounds that are required for the new BRAGFLO Version 6 to calculate the volume of chemical constituents produced or consumed by the previously described chemical reactions. The eight parameters in this group are identified in Tables 1 and 2 by the name REFCON:DN\_XXX. The basis for these parameters is documented in Clayton and Vugrin 2007 [ERMS 545611].

*Group CRA-2009-N2* consists of molecular weights of iron and magnesium compounds that are also required for BRAGFLO Version 6 to calculate the volume of chemical constituents produced or consumed by the previously described chemical reactions. The five parameters in this group are identified in Tables 1 and 2 by the name REFCON:MW\_XXX. The basis for these parameters is documented in Clayton and Vugrin 2007 [ERMS 545611].

*Group CRA-2009-N3* consists of stoichiometric coefficients that are required for BRAGFLO Version 6 to calculate the volume of chemical constituents produced or consumed by the previously described chemical reactions. The stoichiometric coefficients have been organized into a  $7 \times 9$  matrix  $S(I,J)$ , where I represents the reaction and J represents the individual species. A positive value of  $S(I,J)$  represents production and a negative value represents consumption. A zero value generally means that the species is not relevant to the reaction being modeled. For example, the species MgO is not relevant to the anoxic corrosion of iron. The 7 modeled



chemical reactions and 9 chemical species constitute 63 parameters in this group. These parameters are identified in Tables 1 and 2 by the name REFCON:STCO\_ij. The basis for these parameters is documented in Clayton and Vugrin 2007 [ERMS 545611].

*Group CRA-2009-N4* consists of rate constants required for BRAGFLO Version 6 to calculate the extent of MgO hydration. These parameters represent the MgO hydration rate for inundated conditions with Castile brine from WIPP Well ERDA-6, the MgO hydration rate for inundated conditions with Generic Weep Brine (GWB; a synthetic brine representative of grain boundary fluids from the Salado), and the hydration rate for humid conditions. The parameter value for inundated conditions with Castile brine was conservatively set to zero pending completion of current experiments. Because the other two hydration rates were from single experiments, large subjective uncertainties were applied. The three parameters in this group are identified in Tables 1 and 2 by the name WAS\_AREA:BRUCITEx. The basis for these parameters is documented in Deng 2007 [ERMS 545757].

*Group CRA-2009-N5* consists of the single parameter, WAS\_AREA:MGO\_EF. This new parameter is required by BRAGFLO Version 6 to calculate the volume of MgO placed in the repository. The value of this parameter represents the excess of moles of MgO over moles of organic carbon. The basis for these parameters is documented in Clayton and Vugrin 2007 [ERMS 545611].

*Group CRA-2009-N6* consists of the densities of cellulose, plastic, and rubber (CPR) in contact-handled (CH) and remote-handled (RH) waste containers and emplacement materials. These parameters are required by BRAGFLO to calculate the effect of organic carbon in waste containers and emplacement materials on repository gas production and on the MgO excess factor. Contact-handled (CH) emplacement materials contain quantities of cellulose and plastic, while CH emplacement materials contain little rubber. Contact-handled (CH) container materials contain no cellulose or rubber. Remote-handled (RH) container materials contain no cellulose or rubber, and RH emplacement materials contain no cellulose, plastic, or rubber. Materials with little or no CPR are assigned densities of zero. Two related parameters, the density of plastic in CH and RH waste containers (parameters WAS\_AREA:DPLSCCHW and WAS\_AREA:DPLSCRHW), were already in the PAPDB and were used in previous PAs. The 10 parameters in this group are identified in Tables 1 and 2 by the name WAS\_AREA:Dxxx. The basis for these parameters is documented in Nemer 2007b [ERMS 545689].

### **3.1.2 Changed Parameters**

Parameter values that were used in previous PAs and changed for CRA-2009 are classified into seven groups and are described in this section.

*Group CRA-2009-C1* consists of the single parameter, BLOWOUT:MAXFLOW. This constant parameter defines the maximum duration of direct brine releases. Its value was changed from 11 days to 4.5 days, based on distinguishing between blowouts from brine-producing zones and blowouts from gas-producing zones. Gas-producing zones can have longer blowout durations, particularly if a gas fire occurs. The previous maximum blowout duration was based on a 1978 worst-case gas well blowout and fire. The revised value of 4.5 days is based on updated

interviews with area drillers and mud engineers, assuming a maximum repository brine pressure equal to the lithostatic pressure of 14.9 MPa, and including contingencies for possible delays. The basis for this parameter change is documented in Kirkes 2007 [ERMS 545988].

*Group CRA-2009-C2* consists of the single uncertain parameter, BOREHOLE:TAUFAIL. This parameter is assigned a loguniform distribution and defines the effective shear strength for erosion of borehole and fill in an intruding borehole. The lower limit of this distribution was changed from its PABC-2004 value for use in the intermediate AP-131 analysis, and then changed back to its PABC-2004 value for use in the CRA-2009 analysis. As a result, CRA-2009 cavings releases are identical to PABC-2004 releases. These changes in parameter values are documented in Clayton 2007c [ERMS 547515].

*Group CRA-2009-C3* consists of six parameters, four named CAVITY\_x:RELP\_MOD, one named EXP\_AREA:RELP\_MOD, and one named OPS\_AREA:RELP\_MOD. These constant parameters implement a new model, KRP=11, for the capillary pressure and relative permeability of open cavities. This new model removes capillary pressure effects from the calculation of relative permeability. These changes in parameter values are documented in Clayton 2007a [ERMS 545764].

*Group CRA-2009-C4* consists of two parameters, REPOSIT:RELP\_MOD and WAS\_AREA:RELPMOD. These constant parameters implement a new model, KRP=12, for the capillary pressure and relative permeability of waste-filled areas. This new model removes capillary pressure effects from the calculation of relative permeability. These changes in parameter values are documented in Clayton 2007a [ERMS 545764].

*Group CRA-2009-C5* consists of the following four uncertain parameters representing the porosity of Salado halite and the DRZ:

- S\_HALITE:POROSITY, the effective porosity of intact Salado halite
- DRZ\_0:POROSITY, the effective DRZ porosity for time period -5 to 0 years
- DRZ\_1:POROSITY, the effective DRZ porosity for time period 0 to complete healing
- DRZ\_PCS:POROSITY, the effective DRZ porosity above the concrete portion of the panel closure

These new porosity values correct the previous porosity based on weight percent to a porosity based on volume fraction. These parameters are represented by cumulative distributions. Following current WIPP PA practice, these parameter values were determined by increasing S\_HALITE:POROSITY values by 0.0029. These changes in parameter values are documented in Ismail 2007 [ERMS 545755] and Clayton 2007b [ERMS 547486]. In reviewing the source document, EPA found that the change in DRZ porosity was recommended for the parameter DRZ\_2:POROSITY, as well as for the three DRZ porosities listed above. SNL staff explained that the parameter DRZ\_2:POROSITY was not listed as a changed parameter for CRA-2009 because it was created for a postponed 2007 peer review and is not used in compliance calculations.

*Group CRA-2009-C6* consists of one parameter, GLOBAL:LAMBDAD. This constant parameter defines the exploratory borehole drilling rate per unit area in the Delaware Basin. The change in this parameter value represents the increase in drilling rate since PABC-2004, as determined in a 2007 DOE survey. This updated drilling rate is documented in Clayton 2007c [ERMS 547515].

*Group CRA-2009-C7* consists of one parameter, REFCON:FVW. This constant parameter represents the fraction of repository volume occupied by waste. This parameter is calculated by dividing REPOSIT:VOLCHW by REFCON:VREPOS. The value of this parameter was changed twice since the CCA. The value of REFCON:VREPOS was increased in 2002 to account for the volume of three exhaust and intake drifts that were inadvertently excluded from the original calculation. This correction is documented in Stein 2002 [ERMS 523760] and resulted in changing the rounded value of REFCON:FVW from 0.388 to 0.386. A rounding error was subsequently found that changed the revised value of REFCON:FVW from 0.386 to 0.385. This correction is documented in Kirchner 2007 [ERMS 545481]. SNL concluded and EPA concurs that the impact of using the value of 0.386 in PABC-2004 instead of 0.385 is not significant, particularly since it resulted in overestimating the cuttings and spillings releases.

### **3.2 REVIEW OF PAPDB DATABASE-TO-CODE INTERFACE FOR CRA-2009**

Performance assessment (PA) computer codes that execute on the VAX computer platform access the parameter database directly. Accurate access by the WIPP PA codes of PAPDB parameter values was therefore evaluated by comparing code input files with PAPDB database values. The PA code input files were accessed by SNL staff member Dan Clayton in the SNL Carlsbad office. The input files were observed and compared with PAPDB values by the Agency review team. This review was conducted for all parameters used in CRA-2009 that have changed since PABC-2004. The results of this review are shown in Table 3.

Table 3 presents the parameter name (material and property), the code(s) that used the parameter, the names of the input file and library that were accessed, the parameter value in PAPDB, the parameter value returned by the VAX system, and comments providing additional details. For all constant parameters, the value returned was the same as the PAPDB value. For all distributed parameters, the value returned was within the range of the parameter distribution. For distributed parameters, two or more values were generally returned, representing samples for specific vectors randomly selected by the Agency reviewer. Depending on the distributed parameter, vectors representing different replicates, different intrusion scenarios, and different sample times were selected. In addition, the randomly selected MATSET input file for the distributed parameter BOREHOLE:TAUFAIL was reviewed and found to successfully retrieve the median value of this parameter as a placeholder for LHS sampling (see MATSET-LHS interface description in introductory remarks to Section 3.3). The PRELHS files were reviewed for the parameters BOREHOLE:TAUFAIL and S\_HALITE:POROSITY and found to correctly define the proper distributions. The input files for all codes using each parameter were checked and in all cases, a proper value was returned.

**Table 3. Database-Code Interface Test Results for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
BLOWOUT	MAXFLOW	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	3.888E+05	3.888E+05	The correct value was returned.
BOREHOLE	TAUFAIL	CUTTINGS_S	MS_CUSP_CRA-2009.CDB	LIBCRA-2009_CUSP	1.960	1.960	MATSET correctly took the median value as a placeholder.
BOREHOLE	TAUFAIL	CUTTINGS_S	LHS3_CUSP_CRA-2009_R2_V051.CDB	LIBCRA-2009_CUSP	Distributed	2.394	Value from R2 V51. Sampled value correctly lies within sampled range of 0.05 to 77.0.
BOREHOLE	TAUFAIL	CUTTINGS_S	LHS3_CUSP_CRA-2009_R1_V096.CDB	LIBCRA-2009_CUSP	Distributed	28.59	Value from R1 V96. Sampled value correctly lies within sampled range of 0.05 to 77.0.
BOREHOLE	TAUFAIL	PRELHS	LHS1_CRA-2009_R1.TRN	LIBCRA-2009_LHS	Distributed	N/A	PRELHS correctly defined the proper distribution.
CAVITY_1	RELP_MOD	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	11	11	The correct value was returned.
CAVITY_2	RELP_MOD	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	11	11	The correct value was returned.
CAVITY_3	RELP_MOD	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	11	11	The correct value was returned.
CAVITY_4	RELP_MOD	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	11	11	The correct value was returned.
DRZ_0	POROSITY	BRAGFLO	LHS3_BF_CRA-2009_R2_V051.CDB	LIBCRA-2009_BF	Distributed	5.8360E-03	Value from R2 V51. Value populated by adding 2.900E-03 to sampled value of S_HALITE:POROSITY to assure correct correlation. Sampled value correctly lies within sampled range of 3.90E-03 to 5.48E-02.
DRZ_0	POROSITY	BRAGFLO	LHS3_BF_CRA-2009_R1_V096.CDB	LIBCRA-2009_BF	Distributed	1.2016E-02	Value from R1 V96. Value populated by adding 2.900E-03 to sampled value of S_HALITE:POROSITY to assure correct correlation. Sampled value correctly lies within sampled range of 3.90E-03 to 5.48E-02.
DRZ_1	POROSITY	BRAGFLO	LHS3_BF_CRA-2009_R2_V051.CDB	LIBCRA-2009_BF	Distributed	5.8360E-03	Value for R2 V51. Value first calculated for DRZ_0:POROSITY. DRZ_1:POROSITY is then set equal to DRZ_0:POROSITY to assure consistency.
DRZ_1	POROSITY	BRAGFLO	LHS3_BF_CRA-2009_R1_V096.CDB	LIBCRA-2009_BF	Distributed	1.2016E-02	Value for R1 V96. Value first calculated for DRZ_0:POROSITY. DRZ_1:POROSITY is then set equal to DRZ_0:POROSITY to assure consistency.
DRZ_1	POROSITY	BRAGFLO_DBR	REL2_DBR_CRA-2009_R2_S2_T00550_V051.CDB	LIBCRA-2009_DBRR2S2	Distributed	5.8360E-03	Value for R2 S2 T550 V51. Value taken from BRAGFLO output files and mapped to BRAGFLO_DBR input files to assure consistency.
DRZ_1	POROSITY	BRAGFLO_DBR	REL2_DBR_CRA-2009_R1_S3_T01200_V096.CDB	LIBCRA-2009_DBRR1S3	Distributed	1.2016E-02	Value for R1 S3 T1200 V96. Value taken from BRAGFLO output files and mapped to BRAGFLO_DBR input files

**Table 3. Database-Code Interface Test Results for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
							to assure consistency.
DRZ_1	POROSITY	BRAGFLO_DBR	REL2_DBR_CRA-2009_R1_S2_T00550_V096.CDB	LIBCRA-2009_DBR1S2	Distributed	1.2016E-02	Value for R1 S2 T550 V96. Value taken from BRAGFLO output files and mapped to BRAGFLO_DBR input files to assure consistency.
DRZ_PCS	POROSITY	BRAGFLO	LHS3_BF_CRA-2009_R2_V051.CDB	LIBCRA-2009_BF	Distributed	5.8360E-03	Value for R2 V51. Value first calculated for DRZ_0:POROSITY. DRZ_PCS:POROSITY is then set equal to DRZ_0:POROSITY to assure consistency.
DRZ_PCS	POROSITY	BRAGFLO	LHS3_BF_CRA-2009_R1_V096.CDB	LIBCRA-2009_BF	Distributed	1.2016E-02	Value for R1 V96. Value first calculated for DRZ_0:POROSITY. DRZ_PCS:POROSITY is then set equal to DRZ_0:POROSITY to assure consistency.
EXP_AREA	REL_P_MOD	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	11	11	The correct value was returned.
GLOBAL	LAMB_DAD	PRECCDFGF	MS_CCGF_CRA-2009.DBR	LIBCRA-2009_CCGF	5.85E-03	5.85E-03	The correct value was returned.
OPS_AREA	REL_P_MOD	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	11	11	The correct value was returned.
REFCON	DN_CELL	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1100	1100	The correct value was returned.
REFCON	DN_FE	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	7870	7870	The correct value was returned.
REFCON	DN_FEOH2	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	3400	3400	The correct value was returned.
REFCON	DN_FES	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	4700	4700	The correct value was returned.
REFCON	DN_MGCO3	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	3050	3050	The correct value was returned.
REFCON	DN_MGO	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	3600	3600	The correct value was returned.
REFCON	DN_MGOH2	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	2370	2370	The correct value was returned.
REFCON	DN_SALT	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	2180	2180	The correct value was returned.
REFCON	DN_CELL	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	1100	1100	The correct value was returned.
REFCON	DN_FE	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	7870	7870	The correct value was returned.
REFCON	DN_FEOH2	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	3400	3400	The correct value was returned.
REFCON	DN_FES	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	4700	4700	The correct value was returned.
REFCON	DN_MGCO3	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	3050	3050	The correct value was returned.
REFCON	DN_MGO	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	3600	3600	The correct value was returned.
REFCON	DN_MGOH2	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	2370	2370	The correct value was returned.
REFCON	DN_SALT	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	2180	2180	The correct value was returned.
REFCON	FVW	PRECCDFGF	MS_CCGF_CRA-2009.DBR	LIBCRA-2009_CCGF	3.85E-01	3.85E-01	The correct value was returned.
REFCON	MW_FEOH2	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	8.9860E-02	8.9860E-02	The correct value was returned.
REFCON	MW_FES	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	8.7911E-02	8.7911E-02	The correct value was returned.
REFCON	MW_MGCO3	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	8.4314E-02	8.4314E-02	The correct value was returned.
REFCON	MW_MGO	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	4.0304E-02	4.0304E-02	The correct value was returned.
REFCON	MW_MGOH2	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	5.8320E-02	5.8320E-02	The correct value was returned.
REFCON	STCO_11	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1	1	The correct value was returned.
REFCON	STCO_12	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-2	-2	The correct value was returned.
REFCON	STCO_13	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-1	-1	The correct value was returned.

**Table 3. Database-Code Interface Test Results for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
REFCON	STCO_14	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_15	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1	1	The correct value was returned.
REFCON	STCO_16	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_17	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_18	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_19	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_21	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_22	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_23	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_24	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-1	-1	The correct value was returned.
REFCON	STCO_25	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_26	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_27	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_28	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_29	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_31	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-1	-1	The correct value was returned.
REFCON	STCO_32	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	2	2	The correct value was returned.
REFCON	STCO_33	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_34	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_35	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-1	-1	The correct value was returned.
REFCON	STCO_36	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1	1	The correct value was returned.
REFCON	STCO_37	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_38	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_39	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_41	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_42	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_43	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-1	-1	The correct value was returned.
REFCON	STCO_44	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_45	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_46	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1	1	The correct value was returned.
REFCON	STCO_47	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_48	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_49	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_51	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_52	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-1	-1	The correct value was returned.
REFCON	STCO_53	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_54	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_55	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_56	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_57	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-1	-1	The correct value was returned.
REFCON	STCO_58	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1	1	The correct value was returned.
REFCON	STCO_59	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.

**Table 3. Database-Code Interface Test Results for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
REFCON	STCO_61	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_62	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1	1	The correct value was returned.
REFCON	STCO_63	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_64	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_65	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_66	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_67	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_68	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-1	-1	The correct value was returned.
REFCON	STCO_69	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1	1	The correct value was returned.
REFCON	STCO_71	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_72	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_73	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_74	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_75	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_76	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_77	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	-1	-1	The correct value was returned.
REFCON	STCO_78	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
REFCON	STCO_79	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1	1	The correct value was returned.
REPOSIT	RELP_MOD	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	12	12	The correct value was returned.
S_HALITE	POROSITY	BRAGFLO	LHS3_BF_CRA-2009_R2_V051.CDB	LIBCRA-2009_BF	Distributed	2.936E-03	Value from R2 V51. Sampled value correctly lies within sampled range of 1.00E-03 to 5.19E-02.
S_HALITE	POROSITY	BRAGFLO	LHS3_BF_CRA-2009_R1_V096.CDB	LIBCRA-2009_BF	Distributed	9.116E-03	Value from R1 V96. Sampled value correctly lies within sampled range of 1.00E-03 to 5.19E-02.
S_HALITE	POROSITY	BRAGFLO_DBR	REL2_DBR_CRA-2009_R2_S2_T00550_V051.CDB	LIBCRA-2009_DBRR2S2	Distributed	2.936E-03	Value from R2 S2 T550 V51. Sampled value correctly lies within sampled range of 1.00E-03 to 5.19E-02.
S_HALITE	POROSITY	BRAGFLO_DBR	REL2_DBR_CRA-2009_R1_S3_T01200_V096.CDB	LIBCRA-2009_DBRR1S3	Distributed	9.116E-03	Value from R1 S3 T1200 V96. Sampled value correctly lies within sampled range of 1.00E-03 to 5.19E-02.
S_HALITE	POROSITY	BRAGFLO_DBR	REL2_DBR_CRA-2009_R1_S2_T00550_V096.CDB	LIBCRA-2009_DBRR1S2	Distributed	9.116E-03	Value from R1 S2 T550 V96. Sampled value correctly lies within sampled range of 1.00E-03 to 5.19E-02.
S_HALITE	POROSITY	PRELHS	LHS1_CRA-2009_R1.TRN	LIBCRA-2009_LHS	Distributed	N/A	PRELHS correctly defined the proper distribution.
WAS_AREA	BRUCITEC	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
WAS_AREA	BRUCITEH	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	2.10E-09	2.10E-09	The correct value was returned.
WAS_AREA	BRUCITES	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	2.60E-08	2.60E-08	The correct value was returned.
WAS_AREA	MGO_EF	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1.2	1.2	The correct value was returned.
WAS_AREA	DCELCCHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
WAS_AREA	DCELCRHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
WAS_AREA	DCELECHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	1.22	1.22	The correct value was returned.

**Table 3. Database-Code Interface Test Results for Parameters Used in CRA-2009 that have Changed since PABC-2004**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
WAS_AREA	DCELERHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
WAS_AREA	DPLSECHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	8.76	8.76	The correct value was returned.
WAS_AREA	DPLSERHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
WAS_AREA	DRUBCCHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
WAS_AREA	DRUBCRHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
WAS_AREA	DRUBECHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
WAS_AREA	DRUBERHW	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	0	0	The correct value was returned.
WAS_AREA	RELP_MOD	BRAGFLO	MS_BF_CRA-2009.CDB	LIBCRA-2009_BF	12	12	The correct value was returned.
WAS_AREA	RELP_MOD	BRAGFLO_DBR	MS_DBR_CRA-2009.CDB	LIBCRA-2009_DBR	12	12	The correct value was returned.



### 3.3 PA CODE INPUT FILE REVIEW FOR CRA-2009

During EPA's review of PABC-2004, some parameters were found to be hand-coded (manually input) into the files and not drawn from the PAPDB. Therefore, a review of the CRA-2009 PA code input files was conducted to determine if hand-coded parameters remained that, in the opinion of EPA, should have been included in the PAPDB. Using the PAPDB for this purpose is preferred, because it facilitates tracking of parameter value changes and provides a single source for supporting documentation. Because a similar review was conducted for the PABC-2004 input files, the CRA-2009 review focused on the disposition of EPA's previous recommendations and on the changes in input files that have occurred since PABC-2004.

Models and codes used in the CRA-2009 PA were identified in Analysis Plan-137, *Analysis Plan for the Performance Assessment for the 2009 Compliance Recertification Application* (Clayton 2008a [ERMS 547905]). Analysis Plan-137 also identifies new and changed parameters, as well as other changes that have occurred in the analyses since PABC-2004. Analysis Plan-137 states that the CRA-2009 PA used the same radionuclide inventory as was used for PABC-2004, with the addition of the waste emplacement materials, and that no additional inventory calculations were conducted. The CRA-2009 PA calculations performed as a result of updates and corrections involved the following primary codes:

- LHS - Parameter sampling
- BRAGFLO - Salado flow
- PANEL - Actinide mobilization and Salado transport
- NUTS - Salado transport
- MODFLOW - Culebra flow
- SECOTP2D – Culebra transport
- DRSPALL - Spallings releases;
- CUTTINGS\_S - Cuttings and cavings releases
- BRAGFLO\_DBR – Direct brine releases
- CCDFGF - Total release calculations
- STEPWISE - Sensitivity analysis

Three of the primary CRA-2009 PA codes, MODFLOW, SECOTP2D, and DRSPALL, were not changed since PABC-2004. Therefore, the output files for these codes from PABC-2004 were used in the CRA-2009 PA and no new input files were prepared. Data inputs to the PANEL code are used to calculate radionuclide concentrations, which were unchanged from PABC-2004 because the waste inventory remained unchanged. Therefore, no new PANEL input files were prepared for the CRA-2009 PA. STEPWISE is used as a post-processing code for sensitivity analyses of PA results and does not provide direct input to the compliance calculation. The input files for STEPWISE consist of run control parameters and output files from the primary PA codes listed above, and do not require original database parameters. It was not necessary to review the input files for codes that were not changed.

A number of supporting codes are included as subsets of the primary codes listed above. The major supporting codes that require data inputs not derived from other PA codes include

SANTOS (repository porosity), FMT (actinide solubility), GENMESH (mesh generation), MATSET (parameter identification and values), ICSET (initial conditions), ALGEBRA (derived properties), PREBRAG (input files for BRAGFLO), PRELHS (sampled parameter values), and EPAUNI (inventory activities).

Discussions with SNL staff indicated that no new SANTOS calculations were conducted for PABC-2004 or for CRA-2009. Therefore, SANTOS output files from the CCA were used in the CRA-2009 PA. Similarly, the EPAUNI and FMT codes were not rerun, because the waste inventory and actinide solubilities were unchanged since PABC-2004. Input files for these codes were also not reviewed.

The MATSET codes provide input parameter values for many of the primary codes. MATSET identifies the parameters needed for the primary code. It then draws values for the constant parameters and placeholder values (such as the distribution means) for the sampled parameters from the PAPDB. The PRELHS code takes distribution information for all sampled parameters from the PAPDB and provides the information to the LHS code, which selects 100 sampled values for each distributed parameter. These sampled values then replace the placeholder values identified by the MATSET code for the sampled parameters. The PRELHS input files are replicate-specific. One set of these sampled values is used in each realization. Because PRELHS takes distribution information for all sampled parameters and is not specific to a given primary code, its input files are described separately.

This review was conducted by comparing the input files for each of the primary codes identified above that were changed since PABC-2004. Changes in input files were identified using the *difference* command in the VMS operating system. Numerical inputs that were not drawn from the PAPDB, but were hand-coded into the input files, were identified visually and are documented in the following sections. Note that PABC-2004 is identified in the PA input files as CRA1BC. Additional information can be found in the user's manuals for the various codes.

### 3.3.1 BRAGFLO Assessment

BRAGFLO is a two-phase flow code that simulates brine and gas flow in and around the WIPP repository, and incorporates the effects of disposal room closure, gas generation, brine consumption, and inter-bed fracturing in response to gas pressure (Clayton 2008a, Section 2.6.2; ERMS 547905). The following BRAGFLO input files were compared:

GENMESH Input Files:	GM_BF_CRA-2009.INP compared with GM_BF_CRA1BC.INP
MATSET Input Files:	MS_BF_CRA-2009.INP compared with MS_BF_CRA1BC.INP
ICSET Input Files:	IC_BF_CRA-2009.INP compared with IC_BF_CRA1BC.INP
ALGEBRA Input Files:	ALG1_BF_CRA-2009.INP compared with ALG1_BF_CRA1BC.INP ALG2_BF_CRA-2009.INP compared with ALG2_BF_CRA1BC.INP
PREBRAG Input Files:	BF1_CRA-2009_S1.INP compared with BF1_CRA1BC_S1.INP BF1_CRA-2009_S2.INP compared with BF1_CRA1BC_S2.INP

**The GENMESH input file** defines the computational grid framework for the BRAGFLO analyses. No changes in numerical inputs were made since PABC-2004.

**The MATSET input files** for BRAGFLO provides parameter values for the BRAGFLO analyses. Several of the new parameters identified in Section 3.0 above were added to the MATSET input file to account for waste emplacement materials in the inventory, for MgO hydration, and to support the upgrade from BRAGFLO V5.0 to BRAGFLO V6.0. All of these new parameters were taken from the PAPDB. In addition, the hand-coded command PROPERTY\_VALUES, MAT= DRZ\_PCS, NAME\*VALUE: RELP\_MOD = 4.0 in the PABC-2004 input file was removed from the CRA-2009 input file. This parameter is now drawn from the PAPDB in the ALGEBRA input file for BRAGFLO.

**The ICSET input file** establishes initial conditions for the BRAGFLO analyses. The following hand-coded parameter values remain in the CRA-2009 ICSET file for BRAGFLO:

Code lines 39 and 40:            INITIAL\_VALUE, TYPE=ELEMENT, NAME=MGCONC,  
                                  IRANGE=1,69, JRANGE=1,34,& KRANGE=1,2,  
                                  VALUE=0.0

Numerical inputs in the BRAGFLO input file added for CRA-2009 (code lines 39 and 40) identify specific grid blocks and set initial MgO concentrations in those blocks to zero. These values were inserted to assure that no MgO chemical reactions are modeled. EPA does not consider these to be database parameters.

Code lines 88 to 93:            INITIAL\_VALUE, TYPE=ELEMENT, NAME=SATBREL,  
                                  IRANGE=30,30, JRANGE=10,13,& KRANGE=1,2,  
                                  VALUE=DRF\_PCS:SAT\_IBRN  
                                  INITIAL\_VALUE, TYPE=ELEMENT, NAME=SATBREL,  
                                  IRANGE=34,34, JRANGE=10,13,& KRANGE=1,2,  
                                  VALUE=DRF\_PCS:SAT\_IBRN  
                                  INITIAL\_VALUE, TYPE=ELEMENT, NAME=SATBREL,  
                                  IRANGE=38,38, JRANGE=10,13,& KRANGE=1,2,  
                                  VALUE=DRF\_PCS:SAT\_IBRN

These numerical inputs identify specific grid blocks and set initial brine saturations in those blocks to a value taken from the PAPDB. EPA does not consider these run controls to be database parameters.

**Two ALGEBRA files** are used by BRAGFLO. ALGEBRA1 computes derived properties for BRAGFLO that cannot be obtained from the PAPDB. ALGEBRA2 is a post-processor for the results of the BRAGFLO calculations. Changes for CRA-2009 included MgO concentration calculations, modified inventory calculations that include emplaced and container CPR, and modified chemical reaction rate calculations. The parameters that have been removed to the PAPDB or incorporated into other parameters include molecular weights and stoichiometric parameters for corrosion rates.

Excluding unit conversion factors, the following hand-coded parameter values remain in the CRA-2009 ALGEBRA1 input file for BRAGFLO:

Code lines 450 and 451:  $DRH\_RUPL = DRUBBRHW + DRUBCRHW + DRUBERHW +$   
 $\& 1.7*(DPLASRHW + DPLSCRHW + DPLSERHW)$

The factor 1.7 converts the mass of plastic to the equivalent mass of cellulose. The same factor is found in code lines 454 and 455. This factor was also present in the ALGEBRA file for PABC-2004. EPA recommends moving this factor to the PAPDB.

Code line 484:  $WTMGOTOT = (WTCELTOT + TRPLTOT)$   
 $*MGO\_EF*MW\_MGO[B:32]/MW\_CELL[B:32]$

[B:32] is a run control parameter identifying Block 32 in the BRAGFLO input file. This block identifies properties associated with the material REFCON. This and other blocks were also identified in several other code lines and were present in the ALGEBRA1 file for PABC-2004. EPA does not consider these to be database parameters.

Code lines 545 and 546:  $B2 = 10000*DN\_FE[B:32]/MW\_FE[B:32]$   
 $*CORRMCO2[B:30]*\& YRSEC[B:32]*ASDRUM[B:32]$   
 $*DRUMTOT$

The factor 10,000 is the regulatory time frame in years. EPA does not consider this to be a database parameter, because it is unlikely to change.

Code line 591:  $SMIC\_CO2 = MAKEPROP(1.0)$

SMIC\_CO2 is the moles of CO<sub>2</sub> produced per mole of organic carbon. EPA recommends drawing this hand-coded factor from the PAPDB.

Code line 655:  $INTRIN = MAKEPROP(0.0)$

INTRIN is a hand-coded run control parameter that enables the capability to use intrinsic reaction rates for iron, CPR, and MgO. EPA does not consider this to be a database parameter.

Code lines 680 and 695:  $SB\_MIN = 1.05*SAT\_RBRN$

The factor 1.05 is used to calculate minimum brine saturation when using capillary pressure Model 3; otherwise, this factor is not used. This factor was also present in the ALGEBRA1 file for PABC-2004, and was identified in EPA's PABC-2004 parameter review, with the recommendation that it be added to the PAPDB. EPA continues to recommend drawing this factor from the PAPDB.

The hand-coded parameters DIP1 and DIP2 (the dip angle of the Salado Formation in degrees), and CAP\_MOD (the capillary pressure model number) for SHFTU, SHFTL\_T1 and SHFTL\_T2 were also identified in EPA's PABC-2004 parameter review of the ALGEBRA1 file for BRAGFLO, with the recommendation that they be added to the PAPDB. These remained as hand-coded parameters in CRA-2009.

The following hand-coded parameter values remain in the CRA-2009 ALGEBRA2 input file for BRAGFLO:

Code line 164:                   STCO31 = IFEQ0(STCO\_31[B:32],0.0,1.0/  
                                  STCO\_31[B:32])

This code line is used to compute the moles of hydrogen gas per mole of iron hydroxide. The logic statement states that if the value of STCO\_31[B:32] is zero, the value of STCO31 is set to 0.0. If the value of STCO\_31[B:32] is not zero, the value of STCO31 is set to 1.0/STCO\_31[B:32]. Other similar equations are presented on following code lines (for example, code lines 2693 and 3073). EPA does not consider these to be database parameters.

Code lines 192 and 193:        GAS\_C\_V = 0.02463 \* CELL\_MOL  
                                  GAS\_VOL = 0.02463 \* GAS\_MOLE

These equations calculate the volume of gas per mole of gas using a conversion factor of 0.02463. This conversion factor is derived from the standard gas law. Similar code lines were present in the PABC-2004 input file. EPA does not consider this conversion factor to be a database parameter.

Code line 1100:                BRNEAI = BRNEAI + IFLT0(FLOWBRY[E:1234],-  
                                  1.0\*FLOWBRY[E:1235],0.0)

This and other similar equations in following code lines compute cumulative brine flow measured at specific locations. The logic statement states that if the value of FLOWBRY[E:1234] is less than zero (flow is in the Y-direction and is moving down), the value of FLOWBRY[E:1234] is added to BRNEAI. If the value of FLOWBRY[E:1234] is not less than zero, the value of FLOWBRY[E:1234] is not added to BRNEAI. EPA does not consider these to be database parameters.

**The PREBRAG code** prepares input files in a format compatible for BRAGFLO. Separate input files are prepared for Scenario 1 (the undisturbed scenario where no drilling intrusion occurs) and Scenarios 2 through 6 (disturbed scenarios where one or more drilling intrusions occur). The input files for Scenarios 2 through 6 use the same types of numerical inputs, and the file for Scenario 2 was selected by EPA for this review.

Excluding unit conversion factors, the following hand-coded parameter values remain in the CRA-2009 PREBRAG file for Scenario 1:

Code line 36:                   SOLID\_PROD=OFF, MODPERM=1, PERM\_FACTOR=  
                                  WAS\_AREA:PERM\_X, PERM\_EXP = 0.0

Code line 36 has two entries that set numerical flags for PREBRAG Version 8.0. MODPERM is a flag to change the permeability model for the waste area due to creep closure. Setting MODPERM equal to 1 implemented the original PABC-2004 model in CRA-2009. PERM\_EXP is set to zero. PERM\_EXP was also set to zero by a hand entry in the PREBRAG Scenario 1 file for PABC-2004. EPA does not consider these run control parameters to be database parameters.

Code lines 46 to 50:            REGION,MAT=CAVITY\_1, PRES\_BRINE=101325.0,  
                                  SAT\_BRINE=0.0



SCOEFF, MAT= REFCON, TYPE= MGOHR, VAL= 0.0  
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 SCOEFF, MAT= REFCON, TYPE= MGOH2CR, VAL= 0.0  
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 SCOEFF, MAT= REFCON, TYPE= MGOCR, VAL= 0.0  
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

SCOEFF is the matrix of stoichiometric coefficients for all reactions now included in the average stoichiometry model. These hand entries set reactant and product stoichiometries to zero, turning off all chemical reactions except microbial gas production and iron corrosion in the CRA-2009 PA. EPA does not consider these run control parameters to be database parameters.

Code line 345: PERM, TOL=1.0E-2, SOCEFFMIN=1.0E-03

These hand entries are tolerances introduced to prevent singularities (from dividing by zero) when calculating capillary pressure at low saturations in the relative permeability models. TOL applies to Model 11 and SOCEFFMIN applies to Model 12. EPA recommends drawing these values from the PAPDB.

Code lines 706 and 707: DIRICHLET, MAT=MAGENTA, PRESSURE=PRESSURE, &  
 IRANGE=1,1, JRANGE=28,28, KRANGE=1,1

Similar entries are made in code lines 708 through 721. These hand entries are run control parameters that assign materials to specific grid blocks. Similar assignments were made in the PREBRAG Scenario 1 file for PABC-2004. EPA does not consider these run control parameters to be database parameters.

Intrusion Scenario 2 considers a single borehole intrusion at 350 years after repository closure that intersects a Castile brine pocket (called an E1 intrusion). Most of the hand-coded parameter values for PREBRAG Scenario 2 are the same as for PREBRAG Scenario 1, as shown in the following tabulation, and are not duplicated in the following discussion.

<b>Code Lines in PREBRAG Scenario 1</b>	<b>Equivalent Code Lines in PREBRAG Scenario 2</b>
36	36
46 to 50	46 to 50
85 to 134	102 to 182
197	237
313	352
318	357
321 to 325	360 to 364
345	384
706 to 721	783 to 798

The following changes in hand-coded parameter values that are not in PREBRAG Scenario 1 remain in the CRA-2009 PREBRAG file for Scenario 2:

Code line 59 and 60:           BORERESET, NTIME=4, NUM=2,  
                                  MATERIAL=BH\_OPEN, CONC\_PLG, & PRES\_BRIN=-  
                                  1.0, SAT\_BRIN=-1.0, ICHM=1

These hand entries set values for NTIME and NUM. NTIME identifies the time at which the materials change due to a borehole intrusion, and NUM identifies the number of materials to be changed. The iron, MgO, and CPR concentrations are set to zero for the borehole and concrete plug after the borehole intrusion, because they were removed with the borehole cuttings. The -1.0 flag indicates that the brine pressure and saturation are not reset, and the 1 flag indicates that the iron, MgO, and CPR concentrations are changed. EPA does not consider these run control parameters to be database parameters.

Code line 93:                    TIME, TIME\_ID=1, BEGIN= 0.0

Hand entries of this type identify the time at which specific events in Scenario 2 occur in PA. In this entry, ID=1 represents introduction of the waste into the repository and sealing of the shafts at time zero, as measured from repository closure. Other modeled events in PREBRAG Scenario 2 consist of complete salt compaction in the shaft at 200 years (ID=2), the E1 intrusion at 350 years (ID=3), the borehole plugs fail at 550 years (ID=4), and the lower portion of the silty sand borehole filling compacts at 1,550 years (ID=5). These same parameters were entered in the PREBRAG Scenario 2 file for PABC-2004. EPA does not consider these run control parameters to be database parameters.

### 3.3.2 BRAGFLO\_DBR Assessment

The BRAGFLO code is run in the Direct Brine Release (DBR) mode to calculate brine releases from a pressurized repository through an intruding borehole (Clayton 2008a, Section 2.6.7; ERMS 547905). The following BRAGFLO\_DBR input files were compared:

GENMESH Input Files:	GM_DBR_CRA-2009.INP compared with GM_DBR_CRA1BC.INP
MATSET Input Files:	MS_DBR_CRA-2009.INP compared with MS_DBR_CRA1BC.INP
ICSET Input Files:	IC_DBR_CRA-2009_S1.INP compared with IC_DBR_CRA1BC_S1.INP IC_DBR_CRA-2009_S2.INP compared with IC_DBR_CRA1BC_S2.INP
ALGEBRA Input Files:	ALG1_DBR_CRA-2009.INP compared with ALG1_DBR_CRA1BC.INP ALG2_DBR_CRA-2009_S1.INP compared with ALG2_DBR_CRA1BC_S1.INP ALG2_DBR_CRA-2009_S2.INP compared with ALG2_DBR_CRA1BC_S2.INP ALG3_DBR_CRA-2009.INP compared with ALG3_DBR_CRA1BC.INP
RELATE Input Files:	REL1_DBR_CRA-2009.INP compared with REL1_DBR_CRA1BC.INP



REL2\_DBR\_CRA-2009\_S1.INP compared with  
REL2\_DBR\_CRA1BC\_S1.INP  
REL2\_DBR\_CRA-2009\_S2.INP compared with  
REL2\_DBR\_CRA1BC\_S2.INP  
PREBRAG Input Files: BF1\_DBR\_CRA-2009\_S1\_L.INP compared with  
BF1\_DBR\_CRA1BC\_S1\_L.INP  
BF1\_DBR\_CRA-2009\_S1\_M.INP compared with  
BF1\_DBR\_CRA1BC\_S1\_M.INP  
BF1\_DBR\_CRA-2009\_S2\_L.INP compared with  
BF1\_DBR\_CRA1BC\_S2\_L.INP  
BF1\_DBR\_CRA-2009\_S2\_M.INP compared with  
BF1\_DBR\_CRA1BC\_S2\_M.INP

**The GENMESH input file** defines the computational grid framework for the BRAGFLO\_DBR analyses. No changes in numerical inputs were made since PABC-2004.

**The MATSET input files** for BRAGFLO\_DBR provide parameter values for the BRAGFLO\_DBR analyses. No changes in numerical inputs were made since PABC-2004.

**The ICSET input file** establishes initial conditions for the BRAGFLO\_DBR analyses. Separate input files are prepared for Scenario 1 (the undisturbed scenario where no drilling intrusion occurs) and Scenarios 2 through 5 (disturbed scenarios where one drilling intrusion occurs). Five drilling scenarios are used instead of six in this and some subsequent analyses, because Scenario 6 is used to model long-term releases from multiple intrusions. BRAGFLO\_DBR is used to model short-term releases from single intrusions, which only involve Scenarios 1 through 5. The input files for Scenarios 2 through 5 use the same types of numerical inputs, and the file for Scenario 2 was selected by EPA for this review. The following hand-coded parameter value remains in the CRA-2009 ICSET file for BRAGFLO\_DBR Scenario 1:

Code lines 52 and 53: INITIAL\_VALUE, TYPE=ELEMENT, NAME=MGCONC,  
IRANGE=1,40, JRANGE=1,40,& KRANGE=1,2,  
VALUE=0.0

Numerical inputs in the BRAGFLO\_DBR input file added for CRA-2009 (code lines 52 and 53) identify specific grid blocks and set initial MgO concentrations in those blocks to zero. These values were inserted to assure that no MgO chemical reactions are modeled. EPA does not consider these to be database parameters.

Initial MgO concentrations are set to zero in the CRA-2009 ICSET file for BRAGFLO\_DBR Scenario 2 for the same grid blocks as in Scenario 1. The only difference is that code lines 53 and 54 are used in Scenario 2 instead of code lines 52 and 53 in Scenario 1. Again, EPA does not consider these initial values to be database parameters.

**The ALGEBRA files** compute derived properties that cannot be obtained from the PAPDB. There are three different types of ALGEBRA files for BRAGFLO\_DBR. ALGEBRA1 is used to post-process the CUTTINGS\_S code outputs and is not specific to the different drilling scenarios. ALGEBRA2 is used to provide the derived parameters for the BRAGFLO\_DBR

calculations and is specific to the different drilling scenarios. ALGEBRA3 is used to post-process the BRAGFLO\_DBR outputs and is not specific to the different drilling scenarios. No differences were found between the CRA-2009 PA and PABC-2004 involving parameter values in ALGEBRA1. Separate ALGEBRA2 input files are prepared for Scenario 1 (the undisturbed scenario where no drilling intrusion occurs) and Scenarios 2 through 5 (disturbed scenarios where one drilling intrusion occurs). The input files for Scenarios 2 through 5 use the same types of numerical inputs, and the ALGEBRA2 file for Scenario 2 was selected by EPA for this review.

Excluding unit conversion factors, the following hand-coded parameter values remain in the CRA-2009 ALGEBRA2 file for Scenario 1:

Code line 115:  $SB\_MIN = SAT\_RBRN * 1.05$

The factor 1.05 is used to calculate minimum brine saturation when using capillary pressure Model 3; otherwise, this factor is not used. This factor was also present in the ALGEBRA1 file for BRAGFLO and in the ALGEBRA2 file for BRAGFLO\_DBR for PABC-2004. It was identified in EPA's PABC-2004 parameter review, with the recommendation that it be added to the PAPDB. EPA continues to recommend drawing this factor from the PAPDB.

Code lines 126 to 128:  $D1 = MAKEPROP(32.1)$   
 $D2 = MAKEPROP(7.9)$   
 $DE = MAKEPROP(40.0)$

These three parameters are the panel closure dimensions and are repeated in code lines 163 to 165. D1 is the length of the open drift and explosion wall. D2 is the length of the concrete panel closure. DE is the total length. These same parameters are found in the ALGEBRA2 file for the CRA-2004-PABC. EPA recommends moving these parameters to the PAPDB.

Code line 131:  $FACT = MAKEPROP(1.0E10)$

This parameter is a multiplication factor to eliminate round-off errors in very small numbers and is repeated in code line 168. EPA does not consider this to be a database parameter.

Code lines 296 to 298:  $WELLPI\_L = IFGT0(\text{LOG}(\text{DRNRAD\_L}/\text{WELLRAD}) + \text{SKIN} - 0.5, \text{PERM\_X}[\text{ID}:1] * \& \text{HEIGHT}[\text{ID}:1] * 2.0 * \text{PI}[\text{ID}:10] \& / (\text{LOG}(\text{DRNRAD\_L}/\text{WELLRAD}) + \text{SKIN} - 0.5), 1.0)$

The values of 0.5 and 2.0 are constants in the productivity index equation. The value of 1.0 is used as a default value for the well productivity index to avoid dividing by zero. A similar usage appears in code lines 299 to 304. These same values are found in the ALGEBRA2 file for PABC-2004. EPA does not consider these to be database parameters.

Code lines 460 and 461:  $WELPI\_BC = MAKEPROP(0.0)$   
 $BHP\_ABAN = MAKEPROP(0.0)$

These run control parameters set the well productivity index and borehole pressure from a previous intrusion to zero, flagging that no previous intrusion has occurred in this undisturbed scenario. EPA does not consider these to be database parameters.

Intrusion Scenario 2 considers a single borehole intrusion at 350 years after repository closure (called an E1 intrusion). The hand-coded parameter values for ALGEBRA2 Scenario 2 are the same as for ALGEBRA2 Scenario 1, but with different line locations, as shown in the following tabulation. Code lines 460 and 461 in ALGEBRA2 Scenario 1 are not present in ALGEBRA2 Scenario 2.

Code Lines in ALGEBRA 2 Scenario 1	Equivalent Code Lines in ALGEBRA 2 Scenario 2
115	117
126 to 128 and 163 to 165	129 to 131 and 166 to 168
131 and 168	134 and 171
296 to 304	299 to 307

The following hand-coded parameter values remain in the CRA-2009 ALGEBRA3 file:

Code line 62:  $TIMEM = TIME - 1.0$

This equation calculates a modified time that is one second lower to make the integration of brine volume up the borehole correct. This same equation was present in the PABC-2004 input file. EPA does not consider this to be a database parameter.

Code lines 84 and 85:  $BINJ\_REL = MAKEHIST(0.0)$   
 $TMP\_INJ = BINJ\_REL[T:-1]$

These equations are used in calculating the cumulative brine inflow into the repository from a previous intrusion. The value 0.0 in line 84 is used as the initial value for the cumulative volume of brine flowing in the borehole from a previous intrusion. The equation in line 85 sets the value of TMP\_INJ equal to the value of BINJ\_REL at the previous time step. EPA does not consider these to be database parameters.

Code lines 94 and 95:  $BRN\_FLG = TIME/86400.0$   
 $TMP\_FLG = BRN\_FLG[T:-1]$

These equations are used in setting the last time step to be included in a cumulative brine flow calculation. The value 86,400.0 in line 94 converts time in seconds to time in days. The equation in line 95 sets the value of TMP\_FLG equal to the value of BRN\_FLG at the previous time step. EPA does not consider these to be database parameters.

**The RELATE files** provide BRAGFLO\_DBR with the values of calculated properties and sampled parameters developed by the CUTTINGS\_S and BRAGFLO codes. There are two different types of RELATE files for BRAGFLO\_DBR. RELATE1 provides inputs from the CUTTINGS\_S code and RELATE2 provides the BRAGFLO code inputs specific to the different drilling scenarios. Separate input files are prepared for Scenario 1 (the undisturbed scenario where no drilling intrusion occurs) and Scenarios 2 through 5 (disturbed scenarios where one drilling intrusion occurs). The input files for Scenarios 2 through 5 use the same types of

numerical inputs, and the RELATE2 file for Scenario 2 was selected by EPA for this review. No differences were found between the CRA-2009 PA and PABC-2004 involving parameter values in any of the RELATE files.

**The PREBRAG code** prepares input files in a format compatible for BRAGFLO\_DBR. Separate input files are prepared for each combination of drilling scenario and drilling location. Fifteen PREBRAG input files are therefore prepared for BRAGFLO\_DBR to cover the five drilling scenarios and three drilling locations. These input files are essentially the same, and EPA selected the four following files to review: Scenario 1 lower drilling location; Scenario 1 middle drilling location; Scenario 2 lower drilling location; and Scenario 2 middle drilling location. Excluding unit conversion factors, the following hand-coded parameter values remain in the CRA-2009 PREBRAG file for the DBR Scenario 1 lower drilling location input file:

Code line 107:                   TIMES, FILE= ASCII, VALUES= 0.0, 2.592E5, 3.888E5  
This hand entry specifies times at which model outputs are written to file and represent time zero, 3 days (2.592E5 seconds), and 4.5 days (3.888E5 seconds). This code line was changed in the CRA-2009 PA to correspond with reducing the value of BOREHOLE:MAXFLOW, the maximum time for uncontrolled intrusion borehole flow, from 11 to 4.5 days. A similar code line was present in the PREBRAG input file for DBR in PABC-2004. Although these can be considered run control parameters, the maximum time (3.888E5 seconds) is equal to the value of BOREHOLE:MAXFLOW and should be drawn from the PAPDB to assure consistency.

The hand entry identified above on code line 107 for Scenario 1 lower drilling location is also found on code line 107 of the Scenario 1 middle drilling location input file, and on code line 116 for the Scenario 2 lower and middle drilling location input files. No additional CRA-2009 hand entries were identified in these file comparisons.

### 3.3.3 CUTTINGS\_S Assessment

The CUTTINGS\_S code is used to calculate the volume of waste brought to the surface as a result of a borehole that is drilled directly into the repository and penetrates waste containers. The following CUTTINGS\_S input files were compared:

GENMESH Input Files:       GM\_CUSP\_CRA-2009.INP compared with  
  GM\_CUSP\_CRA1BC.INP  
MATSET Input Files:        MS\_CUSP\_CRA-2009.INP compared with  
  MS\_CUSP\_CRA1BC.INP  
CUSP Input Files:         CUSP\_CRA-2009.INP compared with CUSP\_CRA1BC.INP

Note that the CUSP\_CRA1\_S1\_U\_T100.INP input file, reviewed for PABC-2004, is no longer used.

**The GENMESH input file** defines the computational grid framework for the CUTTINGS\_S analyses. No changes in numerical inputs were made since PABC-2004.

**The MATSET input files** provide parameter values for the CUTTINGS\_S analyses. No changes in numerical inputs were made since PABC-2004.

**CUSP** is an input control file for CUTTINGS\_S. No changes in numerical inputs were made since PABC-2004.

### 3.3.4 NUTS Assessment

The NUTS code is used to calculate radionuclide transport through the Salado to the land withdrawal boundary. NUTS uses the same grid as the BRAGFLO code. NUTS requires inputs from BRAGFLO and PANEL, as well as from the PAPDB. NUTS is run in three modes: a screening mode to identify which BRAGFLO vector-scenario combinations are important enough to warrant a full transport analysis; an isotope mode in which a comprehensive transport calculation is made; and an intrusion mode in which intrusion times are simulated that occur at times other than the 350- and 1,000-year intrusions modeled in BRAGFLO. NUTS only simulate scenarios 2 through 5. Transport for Scenario 6 is modeled using the PANEL code. Some of the NUTS inputs are scenario dependent, as indicated below. The following NUTS input files were compared:

NUTS SCN Input Files:	NUT_SCN_CRA-2009_S1.INP compared with NUT_SCN_CRA1BC_S1.INP NUT_SCN_CRA-2009_S2.INP compared with NUT_SCN_CRA1BC_S2.INP
ALGEBRA SCN Input Files:	ALG_NUT_SCN_CRA-2009.INP compared with ALG_NUT_SCN_CRA1BC.INP
NUTS ISO Input Files:	NUT_ISO_CRA-2009_S1.INP compared with NUT_ISO_CRA1BC_S1.INP NUT_ISO_CRA-2009_S2.INP compared with NUT_ISO_CRA1BC_S2.INP
ALGEBRA ISO Input Files:	ALG_NUT_ISO_CRA-2009_S1.INP compared with ALG_NUT_ISO_CRA1BC_S1.INP ALG_NUT_ISO_CRA-2009_S2.INP compared with ALG_NUT_ISO_CRA-2009_S2.INP
NUTS INT Input Files:	NUT_INT_CRA-2009_S2_T00100.INP compared with NUT_INT_CRA1BC_S2_T00100.INP
ALGEBRA INT Input Files:	Uses the ALGEBRA ISO input files (see below)

**The NUTS SCN code** provides a screening analysis to identify vector-scenario combinations that warrant a full transport analysis. NUTS SCN input files are scenario specific. As before, separate input files are prepared for Scenario 1 (the undisturbed scenario where no drilling intrusion occurs) and Scenarios 2 through 5 (disturbed scenarios where one drilling intrusion occurs). The NUTS SCN input files for Scenarios 2 through 5 use the same types of numerical inputs, and the input files for Scenarios 1 and 2 were selected by EPA for this review. No differences were found between the CRA-2009 PA and PABC-2004 involving parameter values in these files.

**The ALGEBRA SCN code** post-processes the NUTS SCN screening run outputs. The ALGEBRA SCN input files are not scenario specific. No differences were found between the CRA-2009 PA and PABC-2004 involving parameter values in these files.

**The NUTS ISO code** calculates radionuclide transport through the Salado to the land withdrawal boundary, and transport through an intrusion borehole and shaft to the Culebra. The NUTS ISO input files are scenario specific, as described above for the NUTS SCN code. The NUTS ISO input files for Scenarios 1 and 2 were selected by EPA for this review. No differences were found between the CRA-2009 PA and PABC-2004 involving parameter values in these files.

**The ALGEBRA ISO code** post-processes the NUTS ISO outputs. The ALGEBRA ISO input files are scenario specific, as described above for the NUTS SCN code. The ALGEBRA ISO input files for Scenarios 1 and 2 were selected by EPA for this review. No differences were found between the CRA-2009 PA and PABC-2004 involving parameter values in these files.

**The NUTS INT code** calculates radionuclide transport through an intrusion borehole and shaft to the Culebra for intrusion times other than the 350- and 1000-year intrusion times modeled in BRAGFLO. The example selected by EPA for review models radionuclide transport for a Scenario 2 borehole intrusion at 100 years that intersects a Castile brine pocket. No differences were found between the CRA-2009 PA and PABC-2004 involving parameter values in this file.

**The ALGEBRA INT code** post-processes the NUTS INT outputs. The requirements for this code are the same as the ALGEBRA ISO code and the ALGEBRA ISO code is used in PA. No differences were found between the CRA-2009 PA and PABC-2004 involving parameter values in this file.

### 3.3.5 CCDFGF Assessment

The CCDFGF code is used to assemble calculated release data from various PA codes into complementary cumulative distribution functions (CCDFs) for comparison with regulatory release limits. EPAUNI is a preprocessor for CCDFGF, but was not rerun for the CRA-2009 PA and, therefore, its input files were not reviewed. The CCDFSUM code reviewed for PABC-2004 was developed to make CCDF plots using CCDFGF outputs, but has been replaced by EXCEL-generated plots and is no longer used. The following CCDFGF input files used in CRA-2009 were compared:

GENMESH Input Files:	GM_CCGF_CRA-2009.INP compared with GM_CCGF_CRA1BC.INP
MATSET Input Files:	MS_CCGF_CRA-2009.INP compared with MS_CCGF_CRA1BC.INP
CONTROL Input Files	CCGF_CRA-2009_CONTROL_R1.INP compared with CCGF_CRA1BC_CONTROL_R1.INP

**The GENMESH input file** defines the single cell mesh used in the CCDFGF calculation. No differences involving parameter values were found between the CRA-2009 PA and PABC-2004 in this file.

**The MATSET input file** provides parameter values for the CCDFGF analyses. No changes in numerical inputs were made since PABC-2004.

**The CONTROL input file** contains CCDFGF run control data. The CONTROL input files for the three replicates calculated in PA are essentially the same. The input file for Replicate 1 was selected by EPA for review. No differences involving parameter values were found between the CRA-2009 PA and PABC-2004 in this file.

### 3.3.6 PRELHS Assessment

As previously explained the PRELHS code takes distribution information for all sampled parameters from the PAPDB and provides the information to the LHS code, which selects 100 sampled values for each distributed parameter. One set of these sampled values is used in each realization. Because PRELHS takes distribution information for all sampled parameters and is not specific to a given primary code, the PRELHS input files are replicate specific. Two of the three replicates, Replicates 1 and 3, were selected by EPA for review. The following PRELHS input files were compared:

PRELHS Input Files: LHS1\_CRA-2009\_R1.INP compared with LHS1\_CRA1BC\_R1.INP  
LHS1\_CRA-2009\_R3.INP compared with LHS1\_CRA1BC\_R3.INP

The following hand-coded parameter value remains in the CRA-2009 PRELHS input file for Replicate 1:

Code line 35:           NOBS 100

This code entry identifies the number of samples of an uncertain parameter in a replicate. The same entry was made in the PRELHS R1 input file for PABC-2004. EPA considers this to be a run control parameter.

This same parameter value was entered on the same code line in the CRA-2009 PRELHS input file for Replicate 3. Again, EPA does not consider this to be a database parameter.

### 3.3.7 Summary of CRA-2009 Input File Review

The focus of EPA's review of the CRA-2009 input files was on changes that occurred since PABC-2004. Identified changes involving hand-coded numerical inputs included both run control parameters and parameters that EPA recommends drawing from the PAPDB. Parameters recommended as being drawn from the PAPDB instead of hand-coding include those with the potential to be changed, for example when implementing sensitivity studies, and those for which traceability to supporting documentation is desirable. References to supporting documentation are an integral part of the PAPDB and provide clear traceability. Referencing supporting documentation can be accomplished as comments within a code, but is not as readily traceable.

The parameters identified in EPA's review of the CRA-2009 input files as recommended for incorporation into the PAPDB are summarized in Table 4. EPA included the list of recommendations in Table 4 in its completeness letter to DOE (Kelly 2009, Issue 3-23-10). DOE's response to these recommendations was included in its 5<sup>th</sup> response submittal to EPA (Moody 2010, Issue 3-23-10) and a summary is included in Table 4.

DOE's response to EPA's parameter recommendations consisted of adding four of the parameters to the PAPDB as new parameters, changing the input file to reference five existing PAPDB parameters instead of hand coding them, modifying the input file to calculate one parameter value instead of hand coding it, identifying five parameters as code configuration parameters that should not be added to the PAPDB, and maintaining one parameter as hand-coded because the input file was not structured to draw that parameter from the PAPDB. EPA accepts this response, recognizing that some parameters fall into a gray area and, if properly traceable, can legitimately be considered code configuration or run control parameters. As previously stated, EPA's principal motivation for recommending adding selected parameters to the PAPDB was to improve traceability. DOE's action has provided adequate traceability by moving some parameters to the PAPDB, by removing the hand coding for those parameters that were already in the PAPDB, and calculating instead of hand coding a parameter. For the six remaining parameters that remain hand-coded, SNL has established adequate traceability as described in Table 4.

### **3.3.8 Summary of EPA CRA-2009 Completeness Issues Related to Parameters**

In accordance with EPA's WIPP Compliance Criteria (40 CFR 194.11), the Agency's full technical evaluation for recertification of the WIPP does not begin until the Agency receives a complete Compliance Recertification Application. As part of this completeness determination, EPA has prepared a series of letters identifying completeness issues and requested DOE to provide responses. Those completeness issues related to parameters and the DOE responses are summarized in Table 5. EPA's completeness issues related to parameters regarded the use of new information in PABC-2009, moving hand-coded parameters from input files to the PAPDB, and correcting a parameter value. EPA has accepted DOE's responses to these issues.



**Table 4. CRA-2009 Hard Coded Inputs Recommended for Incorporation in the PAPDB**

<b>Input File</b>	<b>Code</b>	<b>Parameter Value</b>	<b>Parameter Type</b>	<b>DOE Response</b>	<b>EPA Observation</b>
ALGEBRA1	BRAGFLO	1.7	Factor converting mass of plastic to equivalent mass of cellulosics.	Added to PAPDB as new parameter REFCON:PLASFAC	Response accepted. Traceability is established through the PAPDB.
ALGEBRA1	BRAGFLO	1.0	Moles of CO <sub>2</sub> produced per mole of organic carbon [SMIC_CO2]	Added to PAPDB as new parameter WAS_AREA:SMIC_CO2	Response accepted. Traceability is established through the PAPDB.
ALGEBRA1	BRAGFLO	1.05	Factor to calculate minimum brine saturation when using capillary pressure Model 3	Code configuration parameter, not added to PAPDB	Response accepted. Traceability is provided in the BRAGFLO User's Manual, p. 135 [ERMS 545016]
PREBRAG	BRAGFLO	101325.0	Preclosure brine pressure for Cavities 1 through 4 [PRES_BRINE]	Changed input file to reference existing PAPDB parameter BRINESAL:REF_PRES	Response accepted. Traceability is established through the PAPDB.
PREBRAG	BRAGFLO	0.0	Preclosure brine saturation for Cavities 1 through 4 [SAT_BRINE]	Changed input file to reference existing parameters CAVITY_1:SAT_IBRN CAVITY_2:SAT_IBRN CAVITY_3:SAT_IBRN CAVITY_4:SAT_IBRN	Response accepted. Traceability is established through the PAPDB.
PREBRAG	BRAGFLO	1.5000E-02	Minimum brine saturation cutoff for the waste area [SOCMIN]	Code configuration parameter, not added to PAPDB	Response accepted. Traceability is established through Nemer and Clayton 2008, Section 5.2.2 [ERMS 548607]
PREBRAG	BRAGFLO	1.0E-2	Tolerance for relative permeability Model 11 to prevent singularities when calculating capillary pressure at low saturations [TOL]	Code configuration parameter, not added to PAPDB	Response accepted. Traceability is established through Nemer and Clayton 2008, Section 5.2.7 [ERMS 548607]
PREBRAG	BRAGFLO	1.0E-03	Tolerance for relative permeability Model 12 to prevent singularities when calculating capillary pressure at low saturations [SOCEFFMIN]	Code configuration parameter, not added to PAPDB	Response accepted. Traceability is established through Nemer 2007, p. 56, Equation 130 and associated text discussion [ERMS 545015].
ALGEBRA2	BRAGFLO_DBR	1.05	Factor to calculate minimum brine saturation when using capillary pressure Model 3	Code configuration parameter, not added to PAPDB	Response accepted. Traceability is provided in the BRAGFLO User's Manual, p. 135 [ERMS 545016]
ALGEBRA2	BRAGFLO_DBR	32.1	Panel closure dimension - length of the open drift and explosion wall [D1]	Added to PAPDB as new parameter CONC_PCS:THKOPEN	Response accepted. Traceability is established through the PAPDB.

**Table 4. CRA-2009 Hard Coded Inputs Recommended for Incorporation in the PAPDB**

<b>Input File</b>	<b>Code</b>	<b>Parameter Value</b>	<b>Parameter Type</b>	<b>DOE Response</b>	<b>EPA Observation</b>
ALGEBRA2	BRAGFLO_DBR	7.9	Panel closure dimension - length of the concrete panel closure [D2]	Added to PAPDB as new parameter CONC_PCS:THKCONC	Response accepted. Traceability is established through the PAPDB.
ALGEBRA2	BRAGFLO_DBR	40.0	Panel closure dimension – total length [DE]	Modified the input file to calculate this value from the sum of parameters CONC_PCS:THKOPEN and CONC_PCS:THKCONC	Response accepted. Traceability is established through the PAPDB.
PREBRAG	BRAGFLO_DBR	3.888E5	Maximum time for uncontrolled intrusion borehole flow [TIME]	Although the parameter exists in the PAPDB, PREBRAG version 8.0 only accepts numerical inputs for this output control parameter, and hence the numerical value was maintained in the input file.	Response accepted. Traceability is provided by the following input file comment that immediately precedes the parameter entry: Modified output times to correspond with reduced BOREHOLE:MAXFLOW

**Table 5. Summary of EPA CRA-2009 Completeness Issues Related to Parameters**

EPA Letter Number and Date	EPA Parameter-Related Completeness Issues	DOE Response and Date
#1 5/21/2009	1-23-1 New Compliant Performance Assessment is to use 2008 waste inventory information	1 <sup>st</sup> Response (8/24/2009): The 2008 waste inventory information will be used in PABC-2009.
#1 5/21/2009	1-23-1 New Compliant Performance Assessment is to use new Culebra hydrology model	1 <sup>st</sup> Response (8/24/2009): The new Culebra hydrology model will be used in PABC-2009.
#1 5/21/2009	1-23-1 New Compliant Performance Assessment is to use most recent drilling rate and borehole plugging patterns	1 <sup>st</sup> Response (8/24/2009): The most recent drilling rate and borehole plugging patterns will be used in PABC-2009.
#1 5/21/2009	1-23-3 Evaluate additional solubility uncertainty data	3 <sup>rd</sup> Response (11/25/2009) Updated solubility uncertainties will be used in PABC-2009.
#1 5/21/2009	1-23-4 Evaluate effect of increased ligand concentrations on solubility	1 <sup>st</sup> Response (8/24/2009): Updated solubility values will be used in PABC-2009.
#3 10/19/2009	3-23-10 Certain currently hard coded parameters in the input files should be moved to the PAPDB	5 <sup>th</sup> Response (2/19/2010): A review of the PA input files was conducted and revisions were made as appropriate. *
#3 10/19/2009	3-23-11 The value of the initial waste area pressure is in error and should be corrected.	5 <sup>th</sup> Response (2/19/2010): The initial waste area pressure used in PA is correct. The initial pressure value in Appendix PA-2009 is in error and will be corrected.

\*See section 3.3.7 and Table 4 for EPA's assessment of this response.

References:

- EPA Letter #1: Cotsworth 2009
- EPA Letter #3: Kelly 2009
- DOE Response #1: Moody 2009a
- DOE Response #3: Moody 2009b
- DOE Response #5: Moody 2010

#### **4.0 REVIEW OF PARAMETERS USED IN PABC-2009 THAT HAVE CHANGED SINCE CRA-2009**

This review evaluated 19 new parameters and 130 changes to the values of existing parameters in the PAPDB. These changes were in addition to the parameter changes described in Section 3. The new and changed parameters are identified in Table 6. This table presents the parameter names (consisting of a material name and a property name), the distribution type, the parameter value used in the PABC-2009 analysis, the previous parameter value, the parameter units, and the PA code(s) using the parameter. As before, Parameter Data Entry (PDE) forms provide the source information for parameter values and associated metadata to be entered into the PAPDB. The parameter values and metadata entered into the PAPDB were visually compared with those on the PDE forms and no discrepancies were identified.

Table 7 summarizes an assessment of the adequacy of supporting documentation for justifying the parameter changes. This table provides the parameter name (material and property names), a description of the parameter type, the ERMS numbers for the PDE form and primary supporting document(s), the effective date of the change, and comments that summarize the basis for the change. In each case, the supporting document(s) provided adequate justification for the change. Also in each case, the supporting document(s) were consistent with the values and metadata in the PAPDB.

**Table 6. Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Distribution Type	Parameter Value Used in PABC-2009				Previous Parameter Value				Parameter Units	Used in Code
			Mean	Median	Minimum	Maximum	Mean	Median	Minimum	Maximum		
BOREHOLE	WUF	Constant	2.60	2.60	2.60	2.60	2.32	2.32	2.32	2.32	Curies	PANEL / PRECCDFGF
CAVITY_1	PRESSURE	Constant	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.01325E+05	1.01325E+05	1.01325E+05	1.01325E+05	Pa	BRAGFLO
CAVITY_2	PRESSURE	Constant	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.01325E+05	1.01325E+05	1.01325E+05	1.01325E+05	Pa	BRAGFLO
CONC_MON	CAP_MOD	Constant	1	1	1	1	2	2	2	2	None	BRAGFLO
CONC_MON	PCT_A	Constant	0	0	0	0	5.60E-01	5.60E-01	5.60E-01	5.60E-01	Pa	BRAGFLO
CONC_MON	PCT_EXP	Constant	0	0	0	0	-3.46E-01	-3.46E-01	-3.46E-01	-3.46E-01	None	BRAGFLO
CONC_PCS	CAP_MOD	Constant	1	1	1	1	2	2	2	2	None	BRAGFLO
CONC_PCS	PCT_A	Constant	0	0	0	0	5.60E-01	5.60E-01	5.60E-01	5.60E-01	Pa	BRAGFLO
CONC_PCS	PCT_EXP	Constant	0	0	0	0	-3.46E-01	-3.46E-01	-3.46E-01	-3.46E-01	None	BRAGFLO
CONC_PCS	THKCONC	Constant	7.9	7.9	7.9	7.9	New parameter				m	DBR
CONC_PCS	THKOPEN	Constant	32.1	32.1	32.1	32.1	New parameter				m	DBR
CULEBRA	PRESSURE	Constant	9.333E+05	9.333E+05	9.333E+05	9.333E+05	9.141E+05	9.141E+05	9.141E+05	9.141E+05	Pa	BRAGFLO
CULEBRA	PRMX_LOG	Constant	-14.018	-14.018	-14.018	-14.018	-13.112	-13.112	-13.112	-13.112	log m <sup>2</sup>	BRAGFLO
CULEBRA	PRMY_LOG	Constant	-14.018	-14.018	-14.018	-14.018	-13.112	-13.112	-13.112	-13.112	log m <sup>2</sup>	BRAGFLO
CULEBRA	PRMZ_LOG	Constant	-14.018	-14.018	-14.018	-14.018	-13.112	-13.112	-13.112	-13.112	log m <sup>2</sup>	BRAGFLO
DEWYLAKE	CAP_MOD	Constant	1	1	1	1	2	2	2	2	None	BRAGFLO
DEWYLAKE	PCT_A	Constant	0	0	0	0	2.60E-01	2.60E-01	2.60E-01	2.60E-01	Pa	BRAGFLO
DEWYLAKE	PCT_EXP	Constant	0	0	0	0	-3.48E-01	-3.48E-01	-3.48E-01	-3.48E-01	None	BRAGFLO
DRZ_0	ADDPOR	Constant	0.0029	0.0029	0.0029	0.0029	New parameter				None	BRAGFLO
DRZ_0	DPHIMAX	Constant	0.039	0.039	0.039	0.039	New parameter				None	BRAGFLO
DRZ_0	IFRX	Constant	1	1	1	1	New parameter				None	BRAGFLO
DRZ_0	IFRY	Constant	1	1	1	1	New parameter				None	BRAGFLO
DRZ_0	IFRZ	Constant	0	0	0	0	New parameter				None	BRAGFLO
DRZ_0	KMAXLOG	Constant	-9.0	-9.0	-9.0	-9.0	New parameter				log m <sup>2</sup>	BRAGFLO
DRZ_0	PF_DELTA	Constant	3.8E+06	3.8E+06	3.8E+06	3.8E+06	New parameter				Pa	BRAGFLO
DRZ_0	PI_DELTA	Constant	2.0E+05	2.0E+05	2.0E+05	2.0E+05	New parameter				Pa	BRAGFLO
DRZ_1	EHEIGHT	Constant	43.5	43.5	43.5	43.5	New parameter				m	DBR
GLOBAL	DBRMINBV	Constant	17,400	17,400	17,400	17,400	New parameter				m <sup>3</sup>	PANEL
GLOBAL	LAMBDA	Constant	5.98E-03	5.98E-03	5.98E-03	5.98E-03	5.85E-03	5.85E-03	5.85E-03	5.85E-03	km <sup>-2</sup> yr <sup>-1</sup>	PRECCDFGF

**Table 6. Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Distribution Type	Parameter Value Used in PABC-2009				Previous Parameter Value				Parameter Units	Used in Code
			Mean	Median	Minimum	Maximum	Mean	Median	Minimum	Maximum		
GLOBAL	ONEPLG	Constant	0.022	0.022	0.022	0.022	0.015	0.015	0.015	0.015	None	PRECCDFGF
GLOBAL	THREEPLG	Constant	0.326	0.326	0.326	0.326	0.289	0.289	0.289	0.289	None	PRECCDFGF
GLOBAL	TWOPLG	Constant	0.652	0.652	0.652	0.652	0.696	0.696	0.696	0.696	None	PRECCDFGF
MAGENTA	PRESSURE	Constant	9.631E+05	9.631E+05	9.631E+05	9.631E+05	9.465E+05	9.465E+05	9.465E+05	9.465E+05	Pa	BRAGFLO
MAGENTA	PRMX_LOG	Constant	-14.678	-14.678	-14.678	-14.678	-15.2	-15.2	-15.2	-15.2	log m <sup>2</sup>	BRAGFLO
MAGENTA	PRMY_LOG	Constant	-14.678	-14.678	-14.678	-14.678	-15.2	-15.2	-15.2	-15.2	log m <sup>2</sup>	BRAGFLO
MAGENTA	PRMZ_LOG	Constant	-14.678	-14.678	-14.678	-14.678	-15.2	-15.2	-15.2	-15.2	log m <sup>2</sup>	BRAGFLO
NITRATE	QINIT	Constant	2.79E+07	2.79E+07	2.79E+07	2.79E+07	4.31E+07	4.31E+07	4.31E+07	4.31E+07	moles	BRAGFLO
REFCON	DIP1	Constant	1.0	1.0	1.0	1.0	New parameter				None	BRAGFLO / DBR
REFCON	DIP2	Constant	0.0	0.0	0.0	0.0	New parameter				None	BRAGFLO
REFCON	PLASFAC	Constant	1.7	1.7	1.7	1.7	New parameter				None	BRAGFLO
SHIFTL_T1	CAP_MOD	Constant	1	1	1	1	New parameter				None	BRAGFLO
SHIFTL_T1	PCT_A	Constant	0	0	0	0	5.60E-01	5.60E-01	5.60E-01	5.60E-01	Pa	BRAGFLO
SHIFTL_T1	PCT_EXP	Constant	0	0	0	0	-3.46E-01	-3.46E-01	-3.46E-01	-3.46E-01	None	BRAGFLO
SHIFTL_T2	CAP_MOD	Constant	1	1	1	1	New parameter				None	BRAGFLO
SHIFTL_T2	PCT_A	Constant	0	0	0	0	5.60E-01	5.60E-01	5.60E-01	5.60E-01	Pa	BRAGFLO
SHIFTL_T2	PCT_EXP	Constant	0	0	0	0	-3.46E-01	-3.46E-01	-3.46E-01	-3.46E-01	None	BRAGFLO
SHIFTU	CAP_MOD	Constant	1	1	1	1	New parameter				None	BRAGFLO
SHIFTU	PCT_A	Constant	0	0	0	0	5.60E-01	5.60E-01	5.60E-01	5.60E-01	Pa	BRAGFLO
SHIFTU	PCT_EXP	Constant	0	0	0	0	-3.46E-01	-3.46E-01	-3.46E-01	-3.46E-01	None	BRAGFLO
SOLMOD3	SOLCOH	Constant	1.51E-06	1.51E-06	1.51E-06	1.51E-06	2.88E-07	2.88E-07	2.88E-07	2.88E-07	moles/L	PANEL
SOLMOD3	SOLSOH	Constant	1.66E-06	1.66E-06	1.66E-06	1.66E-06	3.87E-07	3.87E-07	3.87E-07	3.87E-07	moles/L	PANEL
SOLMOD3	SOLVAR	Cumulative	-0.142	0.072	-4.20	2.70	0.035	-0.031	-3.00	2.85	None	PRELHS / PANEL
SOLMOD4	SOLCOH	Constant	6.98E-08	6.98E-08	6.98E-08	6.98E-08	6.79E-08	6.79E-08	6.79E-08	6.79E-08	moles/L	PANEL
SOLMOD4	SOLSOH	Constant	5.63E-08	5.63E-08	5.63E-08	5.63E-08	5.64E-08	5.64E-08	5.64E-08	5.64E-08	moles/L	PANEL
SOLMOD4	SOLVAR	Cumulative	-0.346	-0.520	-2.25	3.30	0.108333	0.075	-1.8	2.4	None	PRELHS / PANEL
SOLMOD5	SOLCOH	Constant	8.75E-07	8.75E-07	8.75E-07	8.75E-07	8.24E-07	8.24E-07	8.24E-07	8.24E-07	moles/L	PANEL
SOLMOD5	SOLSOH	Constant	3.90E-07	3.90E-07	3.90E-07	3.90E-07	3.55E-07	3.55E-07	3.55E-07	3.55E-07	moles/L	PANEL
SULFATE	QINIT	Constant	6.15E+06	6.15E+06	6.15E+06	6.15E+06	4.61E+06	4.61E+06	4.61E+06	4.61E+06	moles	BRAGFLO
WAS_AREA	DCELCHW	Constant	5.10E+00	5.10E+00	5.10E+00	5.10E+00	0	0	0	0	kg/m <sup>3</sup>	BRAGFLO

**Table 6. Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Distribution Type	Parameter Value Used in PABC-2009				Previous Parameter Value				Parameter Units	Used in Code
			Mean	Median	Minimum	Maximum	Mean	Median	Minimum	Maximum		
WAS_AREA	DCELECHW	Constant	1.34E+00	1.34E+00	1.34E+00	1.34E+00	1.22E+00	1.22E+00	1.22E+00	1.22E+00	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DCELLCHW	Constant	4.00E+01	4.00E+01	4.00E+01	4.00E+01	6.00E+01	6.00E+01	6.00E+01	6.00E+01	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DCELLRHW	Constant	2.20E+01	2.20E+01	2.20E+01	2.20E+01	9.30E+00	9.30E+00	9.30E+00	9.30E+00	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DIRNCCHW	Constant	1.90E+02	1.90E+02	1.90E+02	1.90E+02	1.70E+02	1.70E+02	1.70E+02	1.70E+02	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DIRNCRHW	Constant	6.30E+02	6.30E+02	6.30E+02	6.30E+02	5.40E+02	5.40E+02	5.40E+02	5.40E+02	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DIRONCHW	Constant	8.10E+01	8.10E+01	8.10E+01	8.10E+01	1.10E+02	1.10E+02	1.10E+02	1.10E+02	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DIRONRHW	Constant	1.70E+02	1.70E+02	1.70E+02	1.70E+02	5.90E+01	5.90E+01	5.90E+01	5.90E+01	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DPLASCHW	Constant	3.80E+01	3.80E+01	3.80E+01	3.80E+01	4.30E+01	4.30E+01	4.30E+01	4.30E+01	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DPLASRHW	Constant	2.80E+01	2.80E+01	2.80E+01	2.80E+01	8.00E+00	8.00E+00	8.00E+00	8.00E+00	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DPLSCCHW	Constant	1.60E+01	1.60E+01	1.60E+01	1.60E+01	1.70E+01	1.70E+01	1.70E+01	1.70E+01	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DPLSCRHW	Constant	1.40E+01	1.40E+01	1.40E+01	1.40E+01	3.10E+00	3.10E+00	3.10E+00	3.10E+00	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DPLSECHW	Constant	6.59E+00	6.59E+00	6.59E+00	6.59E+00	8.76E+00	8.76E+00	8.76E+00	8.76E+00	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DRUBBCHW	Constant	5.60E+00	5.60E+00	5.60E+00	5.60E+00	1.30E+01	1.30E+01	1.30E+01	1.30E+01	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	DRUBBRHW	Constant	6.60E+00	6.60E+00	6.60E+00	6.60E+00	6.70E+00	6.70E+00	6.70E+00	6.70E+00	kg/m <sup>3</sup>	BRAGFLO
WAS_AREA	SMIC_CO2	Constant	1	1	1	1	New parameter				None	BRAGFLO
AM241	INVCHD	Constant	4.68E+05	4.68E+05	4.68E+05	4.68E+05	5.01E+05	5.01E+05	5.01E+05	5.01E+05	Curies	PANEL
AM241	INVRHD	Constant	4.48E+03	4.48E+03	4.48E+03	4.48E+03	1.65E+04	1.65E+04	1.65E+04	1.65E+04	Curies	PANEL
AM241L	INVCHD	Constant	4.85E+05	4.85E+05	4.85E+05	4.85E+05	5.15E+05	5.15E+05	5.15E+05	5.15E+05	Curies	PANEL
AM241L	INVRHD	Constant	4.61E+03	4.61E+03	4.61E+03	4.61E+03	1.74E+04	1.74E+04	1.74E+04	1.74E+04	Curies	PANEL
AM243	INVCHD	Constant	7.17E+01	7.17E+01	7.17E+01	7.17E+01	7.75E+01	7.75E+01	7.75E+01	7.75E+01	Curies	PANEL
AM243	INVRHD	Constant	7.80E+00	7.80E+00	7.80E+00	7.80E+00	1.13E+00	1.13E+00	1.13E+00	1.13E+00	Curies	PANEL
CF252	INVCHD	Constant	3.28E-02	3.28E-02	3.28E-02	3.28E-02	3.85E-05	3.85E-05	3.85E-05	3.85E-05	Curies	PANEL
CF252	INVRHD	Constant	1.83E-04	1.83E-04	1.83E-04	1.83E-04	1.98E-05	1.98E-05	1.98E-05	1.98E-05	Curies	PANEL
CM243	INVCHD	Constant	1.34E+00	1.34E+00	1.34E+00	1.34E+00	1.82E-01	1.82E-01	1.82E-01	1.82E-01	Curies	PANEL
CM243	INVRHD	Constant	2.09E+00	2.09E+00	2.09E+00	2.09E+00	2.32E-01	2.32E-01	2.32E-01	2.32E-01	Curies	PANEL
CM244	INVCHD	Constant	2.61E+03	2.61E+03	2.61E+03	2.61E+03	1.81E+03	1.81E+03	1.81E+03	1.81E+03	Curies	PANEL
CM244	INVRHD	Constant	4.36E+02	4.36E+02	4.36E+02	4.36E+02	3.20E+02	3.20E+02	3.20E+02	3.20E+02	Curies	PANEL
CM245	INVCHD	Constant	5.86E-01	5.86E-01	5.86E-01	5.86E-01	6.13E-03	6.13E-03	6.13E-03	6.13E-03	Curies	PANEL
CM245	INVRHD	Constant	8.26E-02	8.26E-02	8.26E-02	8.26E-02	1.10E-02	1.10E-02	1.10E-02	1.10E-02	Curies	PANEL
CM248	INVCHD	Constant	1.24E-01	1.24E-01	1.24E-01	1.24E-01	6.51E-02	6.51E-02	6.51E-02	6.51E-02	Curies	PANEL
CM248	INVRHD	Constant	7.63E-03	7.63E-03	7.63E-03	7.63E-03	9.16E-03	9.16E-03	9.16E-03	9.16E-03	Curies	PANEL

**Table 6. Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Distribution Type	Parameter Value Used in PABC-2009				Previous Parameter Value				Parameter Units	Used in Code
			Mean	Median	Minimum	Maximum	Mean	Median	Minimum	Maximum		
CS137	INVCHD	Constant	5.48E+02	5.48E+02	5.48E+02	5.48E+02	3.52E+03	3.52E+03	3.52E+03	3.52E+03	Curies	PANEL
CS137	INVRHD	Constant	8.89E+04	8.89E+04	8.89E+04	8.89E+04	2.03E+05	2.03E+05	2.03E+05	2.03E+05	Curies	PANEL
NP237	INVCHD	Constant	3.65E+01	3.65E+01	3.65E+01	3.65E+01	1.13E+01	1.13E+01	1.13E+01	1.13E+01	Curies	PANEL
NP237	INVRHD	Constant	2.49E+00	2.49E+00	2.49E+00	2.49E+00	8.32E-01	8.32E-01	8.32E-01	8.32E-01	Curies	PANEL
PA231	INVCHD	Constant	3.78E-01	3.78E-01	3.78E-01	3.78E-01	8.69E-01	8.69E-01	8.69E-01	8.69E-01	Curies	PANEL
PA231	INVRHD	Constant	1.87E-01	1.87E-01	1.87E-01	1.87E-01	8.26E-04	8.26E-04	8.26E-04	8.26E-04	Curies	PANEL
PB210	INVCHD	Constant	1.75E+00	1.75E+00	1.75E+00	1.75E+00	3.59E+00	3.59E+00	3.59E+00	3.59E+00	Curies	PANEL
PB210	INVRHD	Constant	1.43E+01	1.43E+01	1.43E+01	1.43E+01	3.02E-05	3.02E-05	3.02E-05	3.02E-05	Curies	PANEL
PM147	INVCHD	Constant	5.09E-02	5.09E-02	5.09E-02	5.09E-02	3.74E-04	3.74E-04	3.74E-04	3.74E-04	Curies	PANEL
PM147	INVRHD	Constant	1.18E+00	1.18E+00	1.18E+00	1.18E+00	1.30E-01	1.30E-01	1.30E-01	1.30E-01	Curies	PANEL
PU238	INVCHD	Constant	1.47E+06	1.47E+06	1.47E+06	1.47E+06	1.13E+06	1.13E+06	1.13E+06	1.13E+06	Curies	PANEL
PU238	INVRHD	Constant	5.11E+03	5.11E+03	5.11E+03	5.11E+03	2.96E+03	2.96E+03	2.96E+03	2.96E+03	Curies	PANEL
PU238L	INVCHD	Constant	1.47E+06	1.47E+06	1.47E+06	1.47E+06	1.13E+06	1.13E+06	1.13E+06	1.13E+06	Curies	PANEL
PU238L	INVRHD	Constant	5.11E+03	5.11E+03	5.11E+03	5.11E+03	2.96E+03	2.96E+03	2.96E+03	2.96E+03	Curies	PANEL
PU239	INVCHD	Constant	5.10E+05	5.10E+05	5.10E+05	5.10E+05	5.77E+05	5.77E+05	5.77E+05	5.77E+05	Curies	PANEL
PU239	INVRHD	Constant	2.92E+03	2.92E+03	2.92E+03	2.92E+03	5.24E+03	5.24E+03	5.24E+03	5.24E+03	Curies	PANEL
PU239L	INVCHD	Constant	6.55E+05	6.55E+05	6.55E+05	6.55E+05	6.71E+05	6.71E+05	6.71E+05	6.71E+05	Curies	PANEL
PU239L	INVRHD	Constant	3.92E+03	3.92E+03	3.92E+03	3.92E+03	6.83E+03	6.83E+03	6.83E+03	6.83E+03	Curies	PANEL
PU240	INVCHD	Constant	1.44E+05	1.44E+05	1.44E+05	1.44E+05	9.38E+04	9.38E+04	9.38E+04	9.38E+04	Curies	PANEL
PU240	INVRHD	Constant	9.89E+02	9.89E+02	9.89E+02	9.89E+02	1.58E+03	1.58E+03	1.58E+03	1.58E+03	Curies	PANEL
PU241	INVCHD	Constant	5.06E+05	5.06E+05	5.06E+05	5.06E+05	4.20E+05	4.20E+05	4.20E+05	4.20E+05	Curies	PANEL
PU241	INVRHD	Constant	3.94E+03	3.94E+03	3.94E+03	3.94E+03	2.80E+04	2.80E+04	2.80E+04	2.80E+04	Curies	PANEL
PU242	INVCHD	Constant	7.46E+01	7.46E+01	7.46E+01	7.46E+01	1.22E+01	1.22E+01	1.22E+01	1.22E+01	Curies	PANEL
PU242	INVRHD	Constant	1.25E+00	1.25E+00	1.25E+00	1.25E+00	4.80E-01	4.80E-01	4.80E-01	4.80E-01	Curies	PANEL
PU244	INVCHD	Constant	3.48E-04	3.48E-04	3.48E-04	3.48E-04	1.26E-06	1.26E-06	1.26E-06	1.26E-06	Curies	PANEL
PU244	INVRHD	Constant	2.34E-06	2.34E-06	2.34E-06	2.34E-06	5.53E-03	5.53E-03	5.53E-03	5.53E-03	Curies	PANEL
RA226	INVCHD	Constant	2.21E+00	2.21E+00	2.21E+00	2.21E+00	4.56E+00	4.56E+00	4.56E+00	4.56E+00	Curies	PANEL
RA226	INVRHD	Constant	1.83E+01	1.83E+01	1.83E+01	1.83E+01	9.34E-05	9.34E-05	9.34E-05	9.34E-05	Curies	PANEL
RA228	INVCHD	Constant	3.08E-01	3.08E-01	3.08E-01	3.08E-01	2.88E+00	2.88E+00	2.88E+00	2.88E+00	Curies	PANEL
RA228	INVRHD	Constant	7.69E-02	7.69E-02	7.69E-02	7.69E-02	1.06E+00	1.06E+00	1.06E+00	1.06E+00	Curies	PANEL
SR90	INVCHD	Constant	5.03E+02	5.03E+02	5.03E+02	5.03E+02	2.62E+04	2.62E+04	2.62E+04	2.62E+04	Curies	PANEL



**Table 6. Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Distribution Type	Parameter Value Used in PABC-2009				Previous Parameter Value				Parameter Units	Used in Code
			Mean	Median	Minimum	Maximum	Mean	Median	Minimum	Maximum		
SR90	INVRHD	Constant	7.99E+04	7.99E+04	7.99E+04	7.99E+04	1.50E+05	1.50E+05	1.50E+05	1.50E+05	Curies	PANEL
TH229	INVCHD	Constant	8.81E+00	8.81E+00	8.81E+00	8.81E+00	4.65E+00	4.65E+00	4.65E+00	4.65E+00	Curies	PANEL
TH229	INVRHD	Constant	4.19E+00	4.19E+00	4.19E+00	4.19E+00	5.64E-01	5.64E-01	5.64E-01	5.64E-01	Curies	PANEL
TH230	INVCHD	Constant	5.87E-01	5.87E-01	5.87E-01	5.87E-01	1.69E-01	1.69E-01	1.69E-01	1.69E-01	Curies	PANEL
TH230	INVRHD	Constant	9.20E-03	9.20E-03	9.20E-03	9.20E-03	1.07E-02	1.07E-02	1.07E-02	1.07E-02	Curies	PANEL
TH230L	INVCHD	Constant	9.40E+00	9.40E+00	9.40E+00	9.40E+00	4.82E+00	4.82E+00	4.82E+00	4.82E+00	Curies	PANEL
TH230L	INVRHD	Constant	4.20E+00	4.20E+00	4.20E+00	4.20E+00	5.75E-01	5.75E-01	5.75E-01	5.75E-01	Curies	PANEL
TH232	INVCHD	Constant	2.75E-01	2.75E-01	2.75E-01	2.75E-01	2.50E+00	2.50E+00	2.50E+00	2.50E+00	Curies	PANEL
TH232	INVRHD	Constant	6.86E-02	6.86E-02	6.86E-02	6.86E-02	9.20E-01	9.20E-01	9.20E-01	9.20E-01	Curies	PANEL
U233	INVCHD	Constant	1.56E+02	1.56E+02	1.56E+02	1.56E+02	1.10E+03	1.10E+03	1.10E+03	1.10E+03	Curies	PANEL
U233	INVRHD	Constant	5.09E+01	5.09E+01	5.09E+01	5.09E+01	1.27E+02	1.27E+02	1.27E+02	1.27E+02	Curies	PANEL
U234	INVCHD	Constant	3.04E+02	3.04E+02	3.04E+02	3.04E+02	3.13E+02	3.13E+02	3.13E+02	3.13E+02	Curies	PANEL
U234	INVRHD	Constant	5.18E+00	5.18E+00	5.18E+00	5.18E+00	3.08E+01	3.08E+01	3.08E+01	3.08E+01	Curies	PANEL
U234L	INVCHD	Constant	4.60E+02	4.60E+02	4.60E+02	4.60E+02	1.41E+03	1.41E+03	1.41E+03	1.41E+03	Curies	PANEL
U234L	INVRHD	Constant	5.61E+01	5.61E+01	5.61E+01	5.61E+01	1.58E+02	1.58E+02	1.58E+02	1.58E+02	Curies	PANEL
U235	INVCHD	Constant	4.42E+00	4.42E+00	4.42E+00	4.42E+00	3.92E+00	3.92E+00	3.92E+00	3.92E+00	Curies	PANEL
U235	INVRHD	Constant	7.04E-02	7.04E-02	7.04E-02	7.04E-02	1.09E+00	1.09E+00	1.09E+00	1.09E+00	Curies	PANEL
U236	INVCHD	Constant	1.35E+00	1.35E+00	1.35E+00	1.35E+00	1.56E+00	1.56E+00	1.56E+00	1.56E+00	Curies	PANEL
U236	INVRHD	Constant	2.48E-01	2.48E-01	2.48E-01	2.48E-01	1.32E+00	1.32E+00	1.32E+00	1.32E+00	Curies	PANEL
U238	INVCHD	Constant	2.71E+01	2.71E+01	2.71E+01	2.71E+01	7.91E+01	7.91E+01	7.91E+01	7.91E+01	Curies	PANEL
U238	INVRHD	Constant	2.96E-01	2.96E-01	2.96E-01	2.96E-01	1.38E+02	1.38E+02	1.38E+02	1.38E+02	Curies	PANEL
AM+3	MKD_AM	Loguniform	0.090	0.045	0.005	0.4	0.13	0.09	0.02	0.4	m <sup>3</sup> /kg	PRELHS / SECOTP2D
NP+4	MKD_NP	Loguniform	1.0	0.071	0.0005	10.0	3.5	2.6	0.7	10.0	m <sup>3</sup> /kg	Not used in PABC-2009
NP+5	MKD_NP	Loguniform	0.023	0.0024	0.00003	0.2	0.038	0.014	0.001	0.2	m <sup>3</sup> /kg	Not used in PABC-2009
PU+3	MKD_PU	Loguniform	0.090	0.045	0.005	0.4	0.13	0.09	0.02	0.4	m <sup>3</sup> /kg	PRELHS / SECOTP2D
PU+4	MKD_PU	Loguniform	1.0	0.071	0.0005	10.0	3.5	2.6	0.7	10.0	m <sup>3</sup> /kg	PRELHS / SECOTP2D
TH+4	MKD_TH	Loguniform	1.0	0.071	0.0005	10.0	3.5	2.6	0.7	10.0	m <sup>3</sup> /kg	PRELHS / SECOTP2D
U+4	MKD_U	Loguniform	1.0	0.071	0.0005	10.0	3.5	2.6	0.7	10.0	m <sup>3</sup> /kg	PRELHS / SECOTP2D

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
BOREHOLE	WUF	Waste Unit Factor: millions of curies of alpha-emitting transuranic radionuclides with half lives greater than 20 years to be disposed at WIPP, decayed to 2033	552242	551679	7/22/2009	This parameter has been updated as shown in Fox et al. (2009, Table B-2). EPA finds this calculated parameter to be appropriate but notes that the information source is incorrectly identified as Table B-1 in the Parameter Data Entry form. Dan Clayton of SNL has agreed to make this correction.
CAVITY_1	PRESSURE	Initial value of brine pore pressure at time zero in cavity for waste areas	552239	551710	7/23/2009	The BRAGFLO MATSET input file has been used to replace the database value of this parameter with a hard coded value since PABC-2004. The hard coded value was larger than the database value and accounted for the increased pressure accumulated in the repository at early time from the fast portion of the microbial gas generation rate. The database value has been replaced by the hard coded value and the value of this parameter is now taken from the database. The revised database value is based on the amount of gas produced at the fast, short-term rate over 481 days and is adequately justified in the secondary source document Nemer et al. (2005, p. 18).
CAVITY_2	PRESSURE	Initial value of brine pore pressure at time zero in cavity for non-waste areas	552239	551710	7/23/2009	Same comment as for CAVITY_1:PRESSURE.
CONC_MON	CAP_MOD	Capillary pressure model number for concrete monolith	552239	551710	7/23/2009	The BRAGFLO ALGEBRA1 input file has been used to replace the database value of this parameter with a hard coded value since the CCA. The hard coded value was used to turn off the capillary pressure model for this material because BRAGFLO would not converge with that model turned on. Although this convergence problem has been corrected in BRAGFLO V6 and the value of this parameter is now taken from the database, the database value was replaced with the formerly hard coded value. The capillary pressure model was therefore not activated in PABC-2009, thereby maintaining consistency with previous PAs. EPA finds the transfer of the hard coded value to the database to be appropriate.
CONC_MON	PCT_A	Threshold pressure linear parameter for capillary pressure model for concrete monolith	552239	551710	7/23/2009	Same comment as for CONC_MON:CAP_MOD.
CONC_MON	PCT_EXP	Threshold pressure exponential parameter for capillary pressure model for concrete monolith	552239	551710	7/23/2009	Same comment as for CONC_MON:CAP_MOD.
CONC_PCS	CAP_MOD	Capillary pressure model number for concrete portion of panel closure system	552239	551710	7/23/2009	The BRAGFLO ALGEBRA1 input file has been used to replace the database value of this parameter with a hard coded value since the CCA. The hard coded value was used to turn off the capillary pressure model for this material because BRAGFLO would not converge with that model turned on. Although this convergence problem has been corrected in BRAGFLO V6 and the value of this parameter is now taken from the database, the

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
						database value was replaced with the formerly hard coded value. The capillary pressure model was therefore not activated in PABC-2009, thereby maintaining consistency with previous PAs. EPA finds the transfer of the hard coded value to the database to be appropriate.
CONC_PCS	PCT_A	Threshold pressure linear parameter for capillary pressure model for concrete portion of panel closure system	552239	551710	7/23/2009	Same comment as for CONC_PCS:CAP_MOD.
CONC_PCS	PCT_EXP	Threshold pressure exponential parameter for capillary pressure model for concrete portion of panel closure system	552239	551710	7/23/2009	Same comment as for CONC_PCS:CAP_MOD.
CONC_PCS	THKCONC	Thickness of panel closure concrete in the Option D panel closure	552247	551715	8/04/2009	New parameter formerly hard coded in the DBR ALGEBRA2 input file. The database value was set equal to the formerly hard coded value. EPA finds this transfer to the database to be appropriate.
CONC_PCS	THKOPEN	Thickness of panel closure empty drift and explosion wall in the Option D panel closure	552247	551715	8/04/2009	Same comment as for CONC_PCS:THKCONC.
CULEBRA	PRESSURE	Brine pore pressure above the WIPP panels in the Culebra member of the Rustler Formation	552241	551646	7/21/2009	The pore pressure was calculated based on the equivalent freshwater head in the Culebra measured in Culebra-Magenta dual completion Well C-2737 in May 2007. This well is located over the center of the WIPP panels. EPA finds this calculation to be appropriate.
CULEBRA	PRMX_LOG	Log of intrinsic permeability, X-direction, in the Culebra member of the Rustler Formation	552241	551646	7/21/2009	The log of the intrinsic permeability in the X-direction was calculated based on the transmissivity and thickness of the Culebra above the WIPP panels. EPA finds this calculation to be appropriate.
CULEBRA	PRMY_LOG	Log of intrinsic permeability, Y-direction, in the Culebra member of the Rustler Formation	552241	551646	7/21/2009	The log of the intrinsic permeability in the Y-direction was set equal to the log of the intrinsic permeability in the X-direction based on the assumption of homogeneity. EPA finds this equivalency to be appropriate.
CULEBRA	PRMZ_LOG	Log of intrinsic permeability, Z-direction, in the Culebra member of the Rustler Formation	552241	551646	7/21/2009	The log of the intrinsic permeability in the Z-direction was set equal to the log of the intrinsic permeability in the X-direction based on the assumption of homogeneity. EPA finds this equivalency to be appropriate.

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
DEWYLAKE	CAP_MOD	Capillary pressure model number for Dewey Lake red beds	552239	551710	7/23/2009	The BRAGFLO ALGEBRA1 input file has been used to replace the database value of this parameter with a hard coded value since the CCA. The hard coded value was used to turn off the capillary pressure model for this material because BRAGFLO would not converge with that model turned on. Although this convergence problem has been corrected in BRAGFLO V6 and the value of this parameter is now taken from the database, the database value was replaced with the formerly hard coded value. The capillary pressure model was therefore not activated in PABC-2009, thereby maintaining consistency with previous PAs. EPA finds the transfer of the hard coded value to the database to be appropriate.
DEWYLAKE	PCT_A	Threshold pressure linear parameter for capillary pressure model for Dewey Lake red beds	552239	551710	7/23/2009	Same comment as for DEWYLAKE:CAP_MOD.
DEWYLAKE	PCT_EXP	Threshold pressure exponential parameter for capillary pressure model for Dewey Lake red beds	552239	551710	7/23/2009	Same comment as for DEWYLAKE:CAP_MOD.
DRZ_0	ADDPOR	Additional porosity in the DRZ caused by fracturing in the time period -5 to 0 years	552238	551710	7/23/2009	New parameter formerly hard coded in the BRAGFLO ALGEBRA1 input file. The database value was set equal to the formerly hard coded value. EPA finds this transfer to the database to be appropriate.
DRZ_0	DPHIMAX	Incremental increase in DRZ porosity relative to intact conditions in the time period -5 to 0 years	552238	551710	7/23/2009	New parameter formerly hard coded in the BRAGFLO ALGEBRA1 input file as equal to the equivalent property for material S_MB139. The database value was set equal to the formerly hard coded value. EPA finds this transfer to the database to be appropriate.
DRZ_0	IFRX	Index for fracture permeability enhancement in the DRZ X-direction in the time period -5 to 0 years	552238	551710	7/23/2009	Same comment as for DRZ_0:DPHIMAX.
DRZ_0	IFRY	Index for fracture permeability enhancement in the DRZ Y-direction in the time period -5 to 0 years	552238	551710	7/23/2009	Same comment as for DRZ_0:DPHIMAX.
DRZ_0	IFRZ	Index for fracture permeability enhancement in the DRZ Z-direction in the time period -5 to 0 years	552238	551710	7/23/2009	Same comment as for DRZ_0:DPHIMAX.
DRZ_0	KMAXLOG	Log of maximum anhydrite permeability in altered anhydrite flow model in the time period -5 to 0 years	552238	551710	7/23/2009	Same comment as for DRZ_0:DPHIMAX.

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
DRZ_0	PF_DELTA	Incremental pressure for full DRZ fracture development in the time period -5 to 0 years	552238	551710	7/23/2009	Same comment as for DRZ_0:DPHIMAX.
DRZ_0	PI_DELTA	DRZ fracture initiation pressure increment in the time period -5 to 0 years	552238	551710	7/23/2009	Same comment as for DRZ_0:DPHIMAX.
DRZ_1	EHEIGHT	Effective height of the DRZ for DBR calculations, beginning at 0 years and ending when DRZ healing is complete	552247	551715	8/04/2009	New parameter formerly hard coded in the DBR MATSET input file. The database value was set equal to the formerly hard coded value. EPA finds this transfer to the database to be appropriate.
GLOBAL	DBRMINBV	Minimum volume of brine in the repository required for a direct brine release	552237	551603	7/21/2009	The minimum brine volume was revised as described in Clayton (2008b) to be consistent with the conceptual model that a DBR will not occur unless the repository pressure exceeds the drilling fluid hydrostatic pressure of 8 MPa. EPA finds this revised value to be appropriate.
GLOBAL	LAMBDA	Drilling rate per unit area	552240	551603	7/21/2009	The deep drilling rate used in PABC-2009 is based on information in the <i>Delaware Basin Monitoring Annual Report</i> (DOE 2008, p. 8), in which a drilling rate of 59.8 boreholes per km <sup>2</sup> was computed over 10,000 years. EPA finds this calculation to be appropriate.
GLOBAL	ONEPLG	Probability of having borehole plug Pattern 1	552240	551603	7/21/2009	The current borehole plugging practices used in PABC-2009 are based on information in the <i>Delaware Basin Monitoring Annual Report</i> (DOE 2008, Table 10). Plug Pattern 1 is represented in the table by Well Type VI, with a current frequency of 2.2%. EPA finds this value to be appropriate.
GLOBAL	THREEPLG	Probability of having borehole plug Pattern 3	552240	551603	7/21/2009	The current borehole plugging practices used in PABC-2009 are based on information in the <i>Delaware Basin Monitoring Annual Report</i> (DOE 2008, Table 10). Plug Pattern 3 is represented in the table by Well Types II and IV, with current frequencies of 20.0% and 12.6%, respectively. EPA finds the total of 32.6% to be appropriate.
GLOBAL	TWOPLG	Probability of having borehole plug Pattern 2	552240	551603	7/21/2009	The current borehole plugging practices used in PABC-2009 are based on information in the <i>Delaware Basin Monitoring Annual Report</i> (DOE 2008, Table 10). Plug Pattern 2 is represented in the table by Well Types I, III, and V, with current frequencies of 29.6%, 32.7%, and 2.9%, respectively. EPA finds the total of 65.2% to be appropriate.
MAGENTA	PRESSURE	Brine pore pressure above the WIPP panels in the Magenta member of the Rustler Formation	552241	551646	7/21/2009	The pore pressure was calculated based on the equivalent freshwater head in the Magenta measured in Culebra-Magenta dual completion Well C-2737 in May 2007. This well is located over the center of the WIPP panels. EPA finds this calculation to be appropriate.
MAGENTA	PRMX_LOG	Log of intrinsic permeability, X-direction, in the Magenta member of the Rustler Formation	552241	551646	7/21/2009	The log of the intrinsic permeability in the X-direction was calculated based on the transmissivity and thickness of the Magenta above the WIPP panels. EPA finds this calculation to be appropriate.

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
MAGENTA	PRMY_LOG	Log of intrinsic permeability, Y-direction, in the Magenta member of the Rustler Formation	552241	551646	7/21/2009	The log of the intrinsic permeability in the Y-direction was set equal to the log of the intrinsic permeability in the X-direction based on the assumption of homogeneity. EPA finds this equivalency to be appropriate.
MAGENTA	PRMZ_LOG	Log of intrinsic permeability, Z-direction, in the Magenta member of the Rustler Formation	552241	551646	7/21/2009	The log of the intrinsic permeability in the Z-direction was set equal to the log of the intrinsic permeability in the X-direction based on the assumption of homogeneity. EPA finds this equivalency to be appropriate.
NITRATE	QINIT	Initial quantity of nitrate in the waste	552245	551679	7/22/2009	This parameter has been updated as shown in Fox et al. (2009, Section 5, p. 16). EPA finds this calculated value to be appropriate.
REFCON	DIP1	Dip angle of the repository toward the panel modeled in BRAGFLO	552238	551710	7/23/2009	New parameter formerly hard coded in the BRAGFLO ALGEBRA1 input file. Value confirmed in secondary source document Helton et al. (1998), p. 4-4. EPA finds this value to be appropriate.
REFCON	DIP2	Dip angle of the Rustler Formation toward the panel modeled in BRAGFLO	552238	551710	7/23/2009	Same comment as for REFCON:DIP1.
REFCON	PLASFAC	Mass ratio of carbon in plastics to carbon in cellulose and rubber	552238	551710	7/23/2009	New parameter formerly hard coded in the BRAGFLO ALGEBRA1 input file. The database value was set equal to the formerly hard coded value. EPA finds this transfer to the database to be appropriate.
SHIFTL_T1	CAP_MOD	Capillary pressure model number for lower portion of simplified shaft from 0 to 200 years	552238	551710	7/23/2009	Same comment as for REFCON:PLASFAC.
SHIFTL_T1	PCT_A	Threshold pressure linear parameter for capillary pressure model for lower portion of simplified shaft from 0 to 200 years	552239	551710	7/23/2009	The BRAGFLO ALGEBRA1 input file has been used to replace the database value of this parameter with a hard coded value since the CCA. The hard coded value was used to turn off the capillary pressure model for this material because BRAGFLO would not converge with that model turned on. Although this convergence problem has been corrected in BRAGFLO V6 and the value of this parameter is now taken from the database, the database value was replaced with the formerly hard coded value. The capillary pressure model was therefore not activated in PABC-2009, thereby maintaining consistency with previous PAs. EPA finds the transfer of the hard coded value to the database to be appropriate.
SHIFTL_T1	PCT_EXP	Threshold pressure exponential parameter for capillary pressure model for lower portion of simplified shaft from 0 to 200 years	552239	551710	7/23/2009	Same comment as for SHIFTL_T1:PCT_A.
SHIFTL_T2	CAP_MOD	Capillary pressure model number for lower portion of simplified shaft from 200 to 10,000 years	552238	551710	7/23/2009	New parameter formerly hard coded in the BRAGFLO ALGEBRA1 input file. The database value was set equal to the formerly hard coded value. EPA finds this transfer to the database to be appropriate.

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
SHIFTL_T2	PCT_A	Threshold pressure linear parameter for capillary pressure model number for lower portion of simplified shaft from 200 to 10,000 years	552239	551710	7/23/2009	The BRAGFLO ALGEBRA1 input file has been used to replace the database value of this parameter with a hard coded value since the CCA. The hard coded value was used to turn off the capillary pressure model for this material because BRAGFLO would not converge with that model turned on. Although this convergence problem has been corrected in BRAGFLO V6 and the value of this parameter is now taken from the database, the database value was replaced with the formerly hard coded value. The capillary pressure model was therefore not activated in PABC-2009, thereby maintaining consistency with previous PAs. EPA finds the transfer of the hard coded value to the database to be appropriate.
SHIFTL_T2	PCT_EXP	Threshold pressure exponential parameter for capillary pressure model number for lower portion of simplified shaft from 200 to 10,000 years	552239	551710	7/23/2009	Same comment as for SHIFTL_T2:PCT_A.
SHIFTU	CAP_MOD	Capillary pressure model number for upper portion of simplified shaft	552238	551710	7/23/2009	New parameter formerly hard coded in the BRAGFLO ALGEBRA1 input file. The database value was set equal to the formerly hard coded value. EPA finds this transfer to the database to be appropriate.
SHIFTU	PCT_A	Threshold pressure linear parameter for capillary pressure model number for upper portion of simplified shaft	552239	551710	7/23/2009	The BRAGFLO ALGEBRA1 input file has been used to replace the database value of this parameter with a hard coded value since the CCA. The hard coded value was used to turn off the capillary pressure model for this material because BRAGFLO would not converge with that model turned on. Although this convergence problem has been corrected in BRAGFLO V6 and the value of this parameter is now taken from the database, the database value was replaced with the formerly hard coded value. The capillary pressure model was therefore not activated in PABC-2009, thereby maintaining consistency with previous PAs. EPA finds the transfer of the hard coded value to the database to be appropriate.
SHIFTU	PCT_EXP	Threshold pressure exponential parameter for capillary pressure model number for upper portion of simplified shaft	552239	551710	7/23/2009	Same comment as for SHIFTU:PCT_A.
SOLMOD3	SOLCOH	Solubility in Castile brine with organics included, controlled by Mg(OH) <sub>2</sub> /hydromagnisite buffer (5424), for Oxidation State III model	552248	552201	10/07/2009	This parameter has been updated as shown in Brush et al. (2009, Table 11, FMT Run 3). EPA finds this calculated value to be appropriate.

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
SOLMOD3	SOLSOH	Solubility in Salado brine with organics included, controlled by Mg(OH) <sub>2</sub> /hydromagnisite buffer (5424), for Oxidation State III model	552248	552201	10/07/2009	This parameter has been updated as shown in Brush et al. (2009, Table 10, FMT Run 5). EPA finds this calculated value to be appropriate.
SOLMOD3	SOLVAR	Solubility uncertainty multiplier for Oxidation State III model	552652	552500	12/01/2009	The distribution for this uncertain parameter has been updated as shown in Xiong et al. (2009, Figure 3 and Table 11), based on differences between measured and predicted solubilities for Neodymium III and Americium III. EPA finds this updated distribution to be appropriate.
SOLMOD4	SOLCOH	Solubility in Castile brine with organics included, controlled by Mg(OH) <sub>2</sub> /hydromagnisite buffer (5424), for Oxidation State IV model	552248	552201	10/07/2009	This parameter has been updated as shown in Brush et al. (2009, Table 11, FMT Run 3). EPA finds this calculated value to be appropriate.
SOLMOD4	SOLSOH	Solubility in Salado brine with organics included, controlled by Mg(OH) <sub>2</sub> /hydromagnisite buffer (5424), for Oxidation State IV model	552248	552201	10/07/2009	This parameter has been updated as shown in Brush et al. (2009, Table 10, FMT Run 5). EPA finds this calculated value to be appropriate.
SOLMOD4	SOLVAR	Solubility uncertainty multiplier for Oxidation State IV model	552652	552500	12/01/2009	The distribution for this uncertain parameter has been updated as shown in Xiong et al. (2009, Figure 1 and Table 7), based on differences between measured and predicted solubilities for Thorium IV. EPA finds this updated distribution to be appropriate.
SOLMOD5	SOLCOH	Solubility in Castile brine with organics included, controlled by Mg(OH) <sub>2</sub> /hydromagnisite buffer (5424), for Oxidation State V model	552248	552201	10/07/2009	This parameter has been updated as shown in Brush et al. (2009, Table 11, FMT Run 3). EPA finds this calculated value to be appropriate.
SOLMOD5	SOLSOH	Solubility in Salado brine with organics included, controlled by Mg(OH) <sub>2</sub> /hydromagnisite buffer (5424), for Oxidation State V model	552248	552201	10/07/2009	This parameter has been updated as shown in Brush et al. (2009, Table 10, FMT Run 5). EPA finds this calculated value to be appropriate.
SULFATE	QINIT	Initial quantity of sulfate in the waste	552245	551679	7/22/2009	This parameter has been updated as shown in Fox et al. (2009, Section 5, p. 16). EPA finds this calculated value to be appropriate.



**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
WAS_AREA	DCELCCHW	Average density of cellulose in contact handled waste container materials	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-4). EPA finds this calculated value to be appropriate.
WAS_AREA	DCELECHW	Average density of cellulose in contact handled waste emplacement materials	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 4-4). EPA finds this calculated value to be appropriate.
WAS_AREA	DCELLCHW	Average density of cellulose in contact handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-4). EPA finds this calculated value to be appropriate.
WAS_AREA	DCELLRHW	Average density of cellulose in remote handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-5). EPA finds this calculated value to be appropriate.
WAS_AREA	DIRNCCHW	Bulk density of iron containers for contact handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-4). EPA finds this calculated value to be appropriate.
WAS_AREA	DIRNCRHW	Bulk density of iron containers for remote handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-5). EPA finds this calculated value to be appropriate.
WAS_AREA	DIRONCHW	Average density of iron-based material in contact handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-4). EPA finds this calculated value to be appropriate.
WAS_AREA	DIRONRHW	Average density of iron-based material in remote handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-5). EPA finds this calculated value to be appropriate.
WAS_AREA	DPLASCHW	Average density of plastics in contact handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-4). EPA finds this calculated value to be appropriate.
WAS_AREA	DPLASRHW	Average density of plastics in remote handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-5). EPA finds this calculated value to be appropriate.
WAS_AREA	DPLSCCHW	Bulk density of plastic liners in contact handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-4). EPA finds this calculated value to be appropriate.
WAS_AREA	DPLSCRHW	Bulk density of plastic liners in remote handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-5). EPA finds this calculated value to be appropriate.
WAS_AREA	DPLSECHW	Average density of plastic in contact handled waste emplacement materials	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 4-4). EPA finds this calculated value to be appropriate.
WAS_AREA	DRUBBCHW	Average density of rubber in contact handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-4). EPA finds this calculated value to be appropriate.
WAS_AREA	DRUBBRHW	Average density of rubber in remote handled waste	552246	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table 5-5). EPA finds this calculated value to be appropriate.

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Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
WAS_AREA	SMIC_CO2	Moles of CO <sub>2</sub> produced per mole of organic carbon consumed in waste emplacement area	552238	551710	7/23/2009	New parameter formerly hard coded in the BRAGFLO ALGEBRA1 input file. This parameter can differ from that in the chemistry stoichiometry matrix because it can be defined differently for different waste areas, although this capability is not currently used. The database value was set equal to the formerly hard coded value. EPA finds this transfer to the database to be appropriate.
AM241	INVCHD	Inventory of Americium 241 in contact handled design	552243	551679	7/22/2009	This parameter has been updated as shown in Crawford et al. (2009, Table A1). EPA finds this calculated value to be appropriate.
AM241	INVRHD	Inventory of Americium 241 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
AM241L	INVCHD	Inventory of Americium 241 lumped with Plutonium 241 in contact handled design	552244	551679	7/22/2009	This parameter has been updated as shown in Fox et al. (2009, Table 5). EPA finds this calculated value to be appropriate.
AM241L	INVRHD	Inventory of Americium 241 lumped with Plutonium 241 in remote handled design	552244	551679	7/22/2009	Same comment as for AM241L:INVCHD
AM243	INVCHD	Inventory of Americium 243 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
AM243	INVRHD	Inventory of Americium 243 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CF252	INVCHD	Inventory of Californium 252 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CF252	INVRHD	Inventory of Californium 252 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CM243	INVCHD	Inventory of Curium 243 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CM243	INVRHD	Inventory of Curium 243 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CM244	INVCHD	Inventory of Curium 244 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CM244	INVRHD	Inventory of Curium 244 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CM245	INVCHD	Inventory of Curium 245 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CM245	INVRHD	Inventory of Curium 245 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CM248	INVCHD	Inventory of Curium 248 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CM248	INVRHD	Inventory of Curium 248 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
CS137	INVCHD	Inventory of Cesium 137 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
CS137	INVRHD	Inventory of Cesium 137 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
NP237	INVCHD	Inventory of Neptunium 237 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
NP237	INVRHD	Inventory of Neptunium 237 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PA231	INVCHD	Inventory of Protactinium 231 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PA231	INVRHD	Inventory of Protactinium 231 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PB210	INVCHD	Inventory of Lead 210 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PB210	INVRHD	Inventory of Lead 210 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PM147	INVCHD	Inventory of Promethium 147 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PM147	INVRHD	Inventory of Promethium 147 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU238	INVCHD	Inventory of Plutonium 238 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU238	INVRHD	Inventory of Plutonium 238 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU238L	INVCHD	Inventory of Plutonium 238 in contact handled design	552244	551679	7/22/2009	Same comment as for AM24L:INVCHD
PU238L	INVRHD	Inventory of Plutonium 238 in remote handled design	552244	551679	7/22/2009	Same comment as for AM24L:INVCHD
PU239	INVCHD	Inventory of Plutonium 239 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU239	INVRHD	Inventory of Plutonium 239 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU239L	INVCHD	Inventory of Plutonium 239 lumped with Plutonium 240 and Plutonium 242 in contact handled design	552244	551679	7/22/2009	Same comment as for AM24L:INVCHD

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
PU239L	INVRHD	Inventory of Plutonium 239 lumped with Plutonium 240 and Plutonium 242 in remote handled design	552244	551679	7/22/2009	Same comment as for AM24L:INVCHD
PU240	INVCHD	Inventory of Plutonium 240 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU240	INVRHD	Inventory of Plutonium 240 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU241	INVCHD	Inventory of Plutonium 241 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU241	INVRHD	Inventory of Plutonium 241 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU242	INVCHD	Inventory of Plutonium 242 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU242	INVRHD	Inventory of Plutonium 242 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU244	INVCHD	Inventory of Plutonium 244 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
PU244	INVRHD	Inventory of Plutonium 244 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
RA226	INVCHD	Inventory of Radium 226 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
RA226	INVRHD	Inventory of Radium 226 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
RA228	INVCHD	Inventory of Radium 228 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
RA228	INVRHD	Inventory of Radium 228 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
SR90	INVCHD	Inventory of Strontium 90 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
SR90	INVRHD	Inventory of Strontium 90 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
TH229	INVCHD	Inventory of Thorium 229 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
TH229	INVRHD	Inventory of Thorium 229 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
TH230	INVCHD	Inventory of Thorium 230 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
TH230	INVRHD	Inventory of Thorium 230 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
TH230L	INVCHD	Inventory of Thorium 230 lumped with Thorium 229 in contact handled design	552244	551679	7/22/2009	Same comment as for AM24L:INVCHD
TH230L	INVRHD	Inventory of Thorium 230 lumped with Thorium 229 in remote handled design	552244	551679	7/22/2009	Same comment as for AM24L:INVCHD
TH232	INVCHD	Inventory of Thorium 232 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
TH232	INVRHD	Inventory of Thorium 232 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U233	INVCHD	Inventory of Uranium 233 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U233	INVRHD	Inventory of Uranium 233 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U234	INVCHD	Inventory of Uranium 234 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U234	INVRHD	Inventory of Uranium 234 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U234L	INVCHD	Inventory of Uranium 234 lumped with Uranium 233 in contact handled design	552244	551679	7/22/2009	Same comment as for AM24L:INVCHD
U234L	INVRHD	Inventory of Uranium 234 lumped with Uranium 233 in remote handled design	552244	551679	7/22/2009	Same comment as for AM24L:INVCHD
U235	INVCHD	Inventory of Uranium 235 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U235	INVRHD	Inventory of Uranium 235 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U236	INVCHD	Inventory of Uranium 236 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U236	INVRHD	Inventory of Uranium 236 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U238	INVCHD	Inventory of Uranium 238 in contact handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
U238	INVRHD	Inventory of Uranium 238 in remote handled design	552243	551679	7/22/2009	Same comment as for AM241:INVCHD
AM+3	MKD_AM	Matrix partition coefficient for Americium III	552443	552395	11/19/2009	This parameter has been updated as shown in Clayton (2009b, Table 2) based on experimental data to account for increased organic ligand concentrations. EPA finds this calculated value to be appropriate.

**Table 7. Justification Check for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Parameter Type	Parameter Data Entry ERMS No.	Supporting Document ERMS No.	Effective Date	Comments
NP+4	MKD_NP	Matrix partition coefficient for Neptunium IV	552443	552395	11/19/2009	This parameter has been updated as shown in Clayton (2009b, Table 3) based on experimental data to account for increased organic ligand concentrations. EPA finds this calculated value to be appropriate.
NP+5	MKD_NP	Matrix partition coefficient for Neptunium V	552443	552395	11/19/2009	This parameter has been updated as shown in Clayton (2009b, Table 4) based on experimental data to account for increased organic ligand concentrations. EPA finds this calculated value to be appropriate.
PU+3	MKD_PU	Matrix partition coefficient for Plutonium III	552443	552395	11/19/2009	This parameter has been updated as shown in Clayton (2009b, Table 5) based on experimental data to account for increased organic ligand concentrations. EPA finds this calculated value to be appropriate.
PU+4	MKD_PU	Matrix partition coefficient for Plutonium IV	552443	552395	11/19/2009	This parameter has been updated as shown in Clayton (2009b, Table 6) based on experimental data to account for increased organic ligand concentrations. EPA finds this calculated value to be appropriate.
TH+4	MKD_TH	Matrix partition coefficient for Thorium IV	552443	552395	11/19/2009	This parameter has been updated as shown in Clayton (2009b, Table 7) based on experimental data to account for increased organic ligand concentrations. EPA finds this calculated value to be appropriate.
U+4	MKD_U	Matrix partition coefficient for Uranium IV	552443	552395	11/19/2009	This parameter has been updated as shown in Clayton (2009b, Table 8) based on experimental data to account for increased organic ligand concentrations. EPA finds this calculated value to be appropriate.

## 4.1 PARAMETER VALUE REVIEW FOR PABC-2009

The results of EPA's PABC-2009 parameter value review are summarized for new parameters in Section 4.1.1 and for existing parameters with changed values in Section 4.1.2.

### 4.1.1 New Parameters

BRAGFLO Version 6.0 (Nemer 2007a [ERMS 545015]) was used in both CRA-2009 and PABC-2009. As explained in Table 7, all new parameters used in PABC-2009 resulted from removing hand-coded values from the PA input files and inserting them into the PAPDB. EPA has classified the new parameters into the following nine groups. Additional information on these parameters is presented in Tables 6 and 7. Because the values of these new parameters are the same as those formerly hand-coded into the input files, they were also used in previous PAs and have been previously reviewed by EPA.

*Group PABC-2009-N1* consists of the down-dip slopes of the repository (DIP1) and the Rustler Formation (DIP2) toward the panel modeled in BRAGFLO. These parameters were formerly hand-coded in the ALGEBRA1 input file for BRAGFLO and were entered into the PAPDB as REFCON:DIP1 and REFCON:DIP2. The basis for these parameters is documented in Nemer 2009 [ERMS 551710] and Helton et al. 1998, p. 4-4 [ERMS 252619].

*Group PABC-2009-N2* consists of a single parameter, the additional porosity in the DRZ caused by fracturing. This parameter was formerly hand-coded in the ALGEBRA1 input file for BRAGFLO and was entered into the PAPDB as DRZ\_0:ADDPOR. The basis for this parameter is documented in Nemer 2009 [ERMS 551710] and Martell 1996 [ERMS 242257].

*Group PABC-2009-N3* consists of seven parameters that account for fracturing in the DRZ. These parameters were formerly hand-coded in the ALGEBRA1 input file for BRAGFLO and were entered into the PAPDB under the material name DRZ 0 and the property names PI\_DELTA; PF\_DELTA; KMAXLOG, DPHIMAX, IFRX; IFRY; and IFRZ. The basis for these parameters is documented in Nemer 2009 [ERMS 551710].

*Group PABC-2009-N4* consists of a single parameter, the mass ratio of carbon in plastics to carbon in cellulose and rubber. This parameter was formerly hand-coded in the ALGEBRA1 input file for BRAGFLO and was entered into the PAPDB as REFCON:PLASFAC. The basis for this parameter is documented in Nemer 2009 [ERMS 551710] and Wang and Brush 1996 [ERMS 231943].

*Group PABC-2009-N5* consists of a single parameter representing the amount of CO<sub>2</sub> produced per mole of organic carbon. The value of this parameter can be different for different waste areas and can therefore be different from the similar parameter in the stoichiometry matrix. This parameter was hand-coded into the ALGEBRA1 input file for BRAGFLO during the CRA-2009 PA as a result of the upgrade from BRAGFLO V5 to BRAGFLO V6 and has been entered into the PAPDB as WAS\_AREA:SMIC\_CO2. The basis for this parameter is documented in Nemer 2009 [ERMS 551710].

*Group PABC-2009-N6* consists of three parameters that identify the capillary pressure model used in BRAGFLO for the shaft materials. These parameters were formerly hand-coded in the ALGEBRA1 input file for BRAGFLO and were entered into the PAPDB under the material names SHIFTL\_T1, SHIFTL\_T2, and SHIFTU, and the property name CAP\_MOD. The basis for these parameters is documented in Nemer 2009 [ERMS 551710] and in the BRAGFLO User's Manual (Nemer 2006, Section 4.9 [ERMS 545016]).

*Group PABC-2009-N7* consists of one parameter, the effective height of the DRZ for DBR calculations. This parameter was formerly hand-coded in the MATSET input file for BRAGFLO\_DBR and was entered into the PAPDB as DRZ\_1:EHEIGHT. The basis for this parameter is documented in Clayton 2009c [ERMS 551715].

*Group PABC-2009-N8* consists of two parameters representing the dimensions of the Option D panel closure for DBR calculations. These parameters were formerly hand-coded in the ALGEBRA2 input file for BRAGFLO\_DBR and were entered into the PAPDB under the material name CONC\_PCS and the property names THKOPEN and THKCONC. The basis for these parameters is documented in Clayton 2009c [ERMS 551715] and in Hadgu et al. 2003, Figure 11 [ERMS 528770].

*Group PABC-2009-N9* consists of a single parameter, the minimum volume of brine in the repository required for a direct brine release. This parameter was formerly hand-coded as the panel-scale minimum brine volume in the MATSET input file for PANEL and was modified to repository-scale and entered into the PAPDB as GLOBAL:DBRMINBV. The basis for this parameter is documented in Clayton 2008b [ERMS 548522].

#### **4.1.2 Changed Parameters**

Parameter values were changed by DOE pursuant to an EPA request that additional information received between the data cutoff for CRA-2009 (December 2007) and the submittal of CRA-2009 (March 2009) be included in an additional PA calculation. The additional information allowed DOE to include updated waste inventory, actinide solubilities and uncertainties, matrix partition coefficients ( $k_d$ s), Culebra transmissivity fields, and drilling parameters in the PABC-2009. EPA did not require the additional chemical capabilities in BRAGFLO Version 6.0, described in Section 3, to be implemented in PABC-2009. Parameter values that were used in previous PAs and changed for PABC-2009 are classified into the following 12 groups. Additional information on these parameters is presented in Tables 6 and 7.

*Group PABC-2009-C1* consists of eight parameters representing brine pressure and permeability in the Culebra and Magenta units of the Rustler Formation. These parameters have the material names CULEBRA and MAGENTA, and the properties PRESSURE, PRMX\_LOG, PRMY\_LOG, and PRMZ\_LOG. These parameters were updated as part of the update of the Culebra transmissivity fields. The PRESSURE values represent the equivalent fresh water brine pressure in each unit in an intrusion borehole over the center of the WIPP waste panels. The pressures are based on May 2007 measurements in Culebra-Magenta dual completion well C-2737 located over the center of the WIPP waste panels. The properties PRMX\_LOG, PRMY\_LOG, and PRMZ\_LOG represent the permeability of the Culebra and Magenta units in



Borehole C-2737. The basis for these parameter changes is documented in Beauheim 2009 [ERMS 551646].

*Group PABC-2009-C2* consists of two parameters representing initial values of repository gas pressure. These parameters are CAVITY\_1:PRESSURE and CAVITY\_2:PRESSURE. CAVITY\_1 is the cavity for waste areas of the repository and CAVITY\_2 is the cavity for non-waste areas. The values of these parameters were changed as part of an SNL review of PA input files. Although these parameters were in the database, the BRAGFLO MATSET input file was hand-coded to replace the database values with higher values to account for the increased pressure accumulated in the repository at early time from the fast portion of the microbial gas generation rate. The database value has been replaced by the hand-coded value and the value of this parameter is now taken from the database. The revised database values are the same for each cavity and are based on the amount of gas produced at the short-term, fast rate over 481 days. The basis for the revised values is documented in Nemer et al. 2005, p. 18 [ERMS 539437].

*Group PABC-2009-C3* consists of 15 parameters that provide input to the capillary pressure model in BRAGFLO. Nine of these parameters have the following material names:

- DEWYLAKE, the Dewey Lake hydrologic unit,
- CONC\_PCS, the concrete portion of Option D panel closure,
- CONC\_MON, the concrete monolith at the bottom of the shaft,

and are associated with the following properties:

- CAP\_MOD, the capillary pressure model number,
- PCT\_A, the threshold pressure linear parameter for capillary pressure model,
- PCT\_EXP, the threshold pressure exponential parameter for capillary pressure model.

The remaining six parameters have the following material names:

- SHFTU, the upper portion of the shaft,
- SHFTL\_T1, the lower portion of the shaft from 0 to 200 years after repository closure,
- SHFTL\_T2, the lower portion of the shaft from 200 to 10,000 years after repository closure,

and are associated with the following properties:

- PCT\_A, the threshold pressure linear parameter for capillary pressure model,
- PCT\_EXP, the threshold pressure exponential parameter for capillary pressure model.

The values of these parameters were changed as part of an SNL review of PA input files. Although these parameters were in the database, the BRAGFLO ALGEBRA1 input file was used to replace the database value of this parameter with a hand-coded value. The hand-coded values were used to turn off the capillary pressure model for these materials because BRAGFLO would not converge with the capillary pressure model turned on. Although this convergence problem has been corrected in BRAGFLO V6 and the values of these parameters are now taken from the database, the database values have been replaced with the formerly hand-coded values. The capillary pressure model therefore remained deactivated in PABC-2009 for these materials, thereby maintaining consistency with previous PAs. The basis for the revised values is documented in Nemer 2006, Section 4.9 [ERMS 545016].

*Group PABC-2009-C4* consists of following four drilling parameters:

- GLOBAL:LAMBDAD, the deep drilling rate per unit area
- GLOBAL:ONEPLG, the probability of having borehole plug Pattern 1
- GLOBAL:TWOPLG, the probability of having borehole plug Pattern 2
- GLOBAL:THREEPLG, the probability of having borehole plug Pattern 3

These parameters are based on surveys of drilling practices in the Delaware Basin and were updated for PABC-2009 based on information in the *Delaware Basin Monitoring Annual Report* (DOE 2008, p. 8 and Table 10).

*Group PABC-2009-C5* consists of one parameter, BOREHOLE:WUF. This parameter is called the Waste Unit Factor or the Unit of Waste. It represents the millions of curies of alpha-emitting transuranic radionuclides with half lives greater than 20 years estimated to be disposed at WIPP, decayed to year 2033. This parameter has been updated as part of the waste inventory update. The basis for the updated value is provided in Fox et al. 2009, Table B-2 [ERMS 551679]. EPA notes that the information source is incorrectly identified as Table B-1 in the BOREHOLE:WUF Parameter Data Entry form [ERMS 552242]. SNL has agreed to correct this error.

*Group PABC-2009-C6* consists of 58 waste inventory parameters with the following material names identifying specific radionuclide isotopes: AM241; AM243; CF252; CM243; CM244; CM245; CM248; CS137; NP237; PA231; PB210; PM147; PU238; PU239; PU240; PU241; PU242; PU244; RA226; RA228; SR90; TH229; TH230; TH232; U233; U234; U235; U236; and U238.

Each of these materials is associated with the following properties:

- INVCHD, the inventory of contact handled waste,
- INVRHD, the inventory of remote handled waste.

Each parameter represents the number of curies of the radionuclide isotope expected to be disposed at WIPP, decayed to year 2033. The updated waste inventory values are based on the *Performance Assessment Inventory Report – 2008* (Crawford et al. 2009 [ERMS 551511]) and are documented in Fox et al. 2009, Table C-2 [ERMS 551679].

*Group PABC-2009-C7* consists of 10 waste inventory parameters with the following material names:

- AM241L, the inventory of Americium 241 lumped with Plutonium 241
- PU238L, the inventory of Plutonium 238 (not lumped)
- PU239L, the inventory of Plutonium 239 lumped with Plutonium 240 and Plutonium 242
- TH230L, the inventory of Thorium 230 lumped with Thorium 229
- U234L, the inventory of Uranium 234 lumped with Uranium 233,

Each of these materials is associated with the following properties:

- INVCHD, the inventory of contact handled waste,
- INVRHD, the inventory of remote handled waste.

Each parameter represents the combined number of curies of the lumped radionuclide isotopes expected to be disposed at WIPP, decayed to year 2033. The updated inventories of these radionuclides were combined to increase the computational efficiency of the PANEL model in

PA. The lumping was justified on the basis that radionuclides of the same elemental form will transport at the same rate. The basis for the lumped values is documented in Fox et al. 2009, Section 4 [ERMS 551679].

*Group PABC-2009-C8* consists of matrix partition coefficient ( $K_d$ ) values for seven following radionuclides:

- AM+3:MKD\_AM, the matrix partition coefficient for Americium III
- NP+4:MKD\_NP, the matrix partition coefficient for Neptunium IV
- NP+5:MKD\_NP, the matrix partition coefficient for Neptunium V
- PU+3:MKD\_PU, the matrix partition coefficient for Plutonium III
- PU+4:MKD\_PU, the matrix partition coefficient for Plutonium IV
- TH+4:MKD\_TH, the matrix partition coefficient for Thorium IV
- U+4:MKD\_U, the matrix partition coefficient for Uranium IV

The  $K_d$  values for these radionuclides were updated as part of the waste inventory update because of a significant increase in the predicted concentrations of organic ligands.

Radionuclides with a given oxidation state are assigned the same  $K_d$  values. These parameters are treated as uncertain in PA and are based on experimental data as described in Clayton 2009b [ERMS 552395].

*Group PABC-2009-C9* consists of the two following parameters:

- NITRATE:QINIT, the initial quantity of nitrate in the waste
- SULFATE:QINIT, the initial quantity of sulfate in the waste

These parameters were updated as part of the waste inventory update. The mass values of these parameters as documented in the *Performance Assessment Inventory Report – 2008* (Crawford et al. 2009 [ERMS 551511]) were converted to moles for input to PABC-2009, as documented in Fox et al. 2009, Section 5 [ERMS 551679].

*Group PABC-2009-C10* consists of 15 parameters with the material name WAS-AREA and the property names DIRONCHW, DIRONRHW, DIRNCCHW, DIRNCRHW, DCELLCHW, DCELLRHW, DCELCCHW, DCELECHW, DPLASCHW, DPLASRHW, DPLSCCHW, DPLSCRHW, DPLSECHW, DRUBBCHW, and DRUBBRHW. These parameter values were updated as part of the waste inventory update and represent the average densities of iron, cellulose, plastics, and rubber in contact and remote handled waste, waste packaging materials, waste emplacement materials, and waste containers disposed in the WIPP repository. These parameter values are documented in the *Performance Assessment Inventory Report – 2008* (Crawford et al. 2009, Table 5-4 [ERMS 551511]) and in Fox et al. 2009, Table C-4 [ERMS 551679].

*Group PABC-2009-C11* consists of six parameters with the following material names:

- SOLMOD3, the Oxidation State III model
- SOLMOD4, the Oxidation State IV model
- SOLMOD5, the Oxidation State V model

Each of these materials is associated the following properties:

- SOLSOH, the solubility in Salado brine with organics included, controlled by  $Mg(OH)_2$ /hydromagnisite buffer (5424)
- SOLCOH, the solubility in Castile brine with organics included, controlled by  $Mg(OH)_2$ /hydromagnisite buffer (5424)

These parameters represent waste solubilities and have been updated based on FMT model runs that account for the updated waste inventory and WIPP repository conditions. The basis for the updated values is described in Brush et al. 2009; Table 10, FMT Run 5 for Salado brine, and Table 11, FMT Run 3 for Castile brine [ERMS 552201]. The other FMT runs were used for sensitivity analyses.

*Group PABC-2009-C12* consists of the following two parameters:

- SOLMOD3:SOLVAR, the solubility uncertainty multiplier for Oxidation State III model
- SOLMOD4:SOLVAR, the solubility uncertainty multiplier for Oxidation State IV model

These uncertain parameters represent the uncertainty in waste solubilities and were updated based on incorporating more recent experimental results into the analysis. The distribution for SOLMOD3:SOLVAR has been updated as described in Xiong et al. (2009, Figure 3 and Table 11 [ERMS 552500]), based on differences between measured and predicted solubilities for Neodymium III and Americium III. The distribution for SOLMOD4:SOLVAR has been updated as shown in Xiong et al. (2009, Figure 1 and Table 7 [ERMS 552500]), based on differences between measured and predicted solubilities for Thorium IV.

## **4.2 REVIEW OF PAPDB DATABASE-TO-CODE INTERFACE FOR PABC-2009**

Performance assessment (PA) computer codes that execute on the VAX computer platform access the parameter database directly. Accurate access by those WIPP PA codes of PAPDB parameter values was therefore evaluated by comparing code input files with PAPDB database values. The PA code input files were accessed by SNL staff member Dan Clayton in the SNL Carlsbad office. The input files were observed and compared with PAPDB values by the Agency review team. This review was conducted for all parameters used in PABC-2009 that are new or have been changed since CRA-2009. The results of this review are shown in Table 8.

Table 8 presents the parameter name (material and property), the code(s) that used the parameter, the names of the input file and library that were accessed, the parameter value in PAPDB, the parameter value returned by the VAX system, and comments providing additional details. For all constant parameters, the value returned was the same as the PAPDB value. For all distributed parameters, the value returned was within the range of the parameter distribution. For distributed parameters, two values were generally returned as a check, representing samples for specific replicates randomly selected by the Agency reviewer. Depending on the distributed parameter, vectors representing specific replicates and vectors were also randomly selected. In addition, the MATSET input files for the distributed parameters were reviewed and found to successfully retrieve the median value of the parameters as placeholders for LHS sampling (see MATSET-LHS interface description in introductory remarks to Section 3.3). The PRELHS files (LHS1) were reviewed and found to correctly define the proper distributions. The POSTLHS

files (LHS3) were reviewed and found to correctly return parameter values within the sampled range. The input files for all codes using each parameter were checked and in all cases, a proper value was returned.

**Table 8. Database-Code Interface Test Results for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
BOREHOLE	WUF	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	2.60	2.60	The correct value was returned
BOREHOLE	WUF	PRECCDFGF	MS_CCGF_PABC-2009.CDB	LIBPABC-2009_CCGF	2.60	2.60	The correct value was returned
CAVITY_1	PRESSURE	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1.28039E+05	1.28039E+05	The correct value was returned
CAVITY_2	PRESSURE	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1.28039E+05	1.28039E+05	The correct value was returned
CONC_MON	CAP_MOD	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1	1	The correct value was returned
CONC_MON	PCT_A	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
CONC_MON	PCT_EXP	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
CONC_PCS	CAP_MOD	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1	1	The correct value was returned
CONC_PCS	PCT_A	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
CONC_PCS	PCT_EXP	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
CONC_PCS	THKCONC	DBR	MS_DBR_PABC-2009.CDB	LIBPABC-2009_DBR	7.9	7.9	The correct value was returned
CONC_PCS	THKOPEN	DBR	MS_DBR_PABC-2009.CDB	LIBPABC-2009_DBR	32.1	32.1	The correct value was returned
CULEBRA	PRESSURE	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	9.333E+05	9.333E+05	The correct value was returned
CULEBRA	PRMX_LOG	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	-14.018	-14.018	The correct value was returned
CULEBRA	PRMY_LOG	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	-14.018	-14.018	The correct value was returned
CULEBRA	PRMZ_LOG	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	-14.018	-14.018	The correct value was returned
DEWYLAKE	CAP_MOD	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1	1	The correct value was returned
DEWYLAKE	PCT_A	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
DEWYLAKE	PCT_EXP	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
DRZ_0	ADDPOR	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0.0029	0.0029	The correct value was returned
DRZ_0	DPHIMAX	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0.039	0.039	The correct value was returned
DRZ_0	IFRX	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1	1	The correct value was returned
DRZ_0	IFRY	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1	1	The correct value was returned
DRZ_0	IFRZ	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
DRZ_0	KMAXLOG	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	-9.0	-9.0	The correct value was returned
DRZ_0	PF_DELTA	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	3.8E+06	3.8E+06	The correct value was returned
DRZ_0	PI_DELTA	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	2.0E+05	2.0E+05	The correct value was returned
DRZ_1	EHEIGHT	DBR	MS_DBR_PABC-2009.CDB	LIBPABC-2009_DBR	43.5	43.5	The correct value was returned
GLOBAL	DBRMINBV	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	17,400	17,400	The correct value was returned
GLOBAL	LAMBDA	PRECCDFGF	MS_CCGF_PABC-2009.CDB	LIBPABC-2009_CCGF	5.98E-03	5.98E-03	The correct value was returned
GLOBAL	ONEPLG	PRECCDFGF	MS_CCGF_PABC-2009.CDB	LIBPABC-2009_CCGF	0.022	0.022	The correct value was returned
GLOBAL	THREEPLG	PRECCDFGF	MS_CCGF_PABC-2009.CDB	LIBPABC-2009_CCGF	0.326	0.326	The correct value was returned
GLOBAL	TWOPLG	PRECCDFGF	MS_CCGF_PABC-2009.CDB	LIBPABC-2009_CCGF	0.652	0.652	The correct value was returned
MAGENTA	PRESSURE	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	9.631E+05	9.631E+05	The correct value was returned

**Table 8. Database-Code Interface Test Results for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
MAGENTA	PRMX_LOG	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	-14.678	-14.678	The correct value was returned
MAGENTA	PRMY_LOG	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	-14.678	-14.678	The correct value was returned
MAGENTA	PRMZ_LOG	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	-14.678	-14.678	The correct value was returned
NITRATE	QINIT	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	2.79E+07	2.79E+07	The correct value was returned
REFCON	DIP1	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1.0	1.0	The correct value was returned
REFCON	DIP1	BRAGFLO_DBR	MS_DBR_PABC-2009.CDB	LIBPABC-2009_DBR	1.0	1.0	The correct value was returned
REFCON	DIP2	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0.0	0.0	The correct value was returned
REFCON	PLASFAC	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1.7	1.7	The correct value was returned
SHIFTL_T1	CAP_MOD	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1	1	The correct value was returned
SHIFTL_T1	PCT_A	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
SHIFTL_T1	PCT_EXP	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
SHIFTL_T2	CAP_MOD	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1	1	The correct value was returned
SHIFTL_T2	PCT_A	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
SHIFTL_T2	PCT_EXP	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
SHIFTU	CAP_MOD	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1	1	The correct value was returned
SHIFTU	PCT_A	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
SHIFTU	PCT_EXP	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	0	0	The correct value was returned
SOLMOD3	SOLCOH	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	1.51E-06	1.51E-06	The correct value was returned
SOLMOD3	SOLSOH	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	1.66E-06	1.66E-06	The correct value was returned
SOLMOD3	SOLVAR	PRELHS	LHS1_PABC-2009_R1.TRN	LIBPABC-2009_LHS	Distributed	Distributed	Probabilities are listed as cumulative values in the PAPDB and are converted to differences between cumulative values in the PRELHS input file. The conversion was checked and found to be accurate for Replicate 1.
SOLMOD3	SOLVAR	PRELHS	LHS1_PABC-2009_R3.TRN	LIBPABC-2009_LHS	Distributed	Distributed	Probabilities are listed as cumulative values in the PAPDB and are converted to differences between cumulative values in the PRELHS input file. The conversion was checked and found to be accurate for Replicate 3.
SOLMOD3	SOLVAR	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	0.072	0.072	MATSET correctly took the median value as a placeholder
SOLMOD3	SOLVAR	PANEL	LHS3_PANEL_PABC-2009_R2_V031.CDB	LIBPABC-2009_PANEL	Distributed	2.567	Value from R2 V31. Sampled value correctly lies within sampled range of -4.20 to 2.70.
SOLMOD4	SOLCOH	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	6.98E-08	6.98E-08	The correct value was returned

**Table 8. Database-Code Interface Test Results for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
SOLMOD4	SOLSOH	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	5.63E-08	5.63E-08	The correct value was returned
SOLMOD4	SOLVAR	PRELHS	LHS1_PABC-2009_R1.TRN	LIBPABC-2009_LHS	Distributed	Distributed	Probabilities are listed as cumulative values in the PAPDB and are converted to differences between cumulative values in the PRELHS input file. The conversion was checked and found to be accurate for Replicate 1.
SOLMOD4	SOLVAR	PRELHS	LHS1_PABC-2009_R3.TRN	LIBPABC-2009_LHS	Distributed	Distributed	Probabilities are listed as cumulative values in the PAPDB and are converted to differences between cumulative values in the PRELHS input file. The conversion was checked and found to be accurate for Replicate 3.
SOLMOD4	SOLVAR	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	-0.520	-0.520	MATSET correctly took the median value as a placeholder
SOLMOD4	SOLVAR	PANEL	LHS3_PANEL_PABC-2009_R2_V031.CDB	LIBPABC-2009_PANEL	Distributed	0.2418	Value from R2 V31. Sampled value correctly lies within sampled range of -2.25 to 3.30.
SOLMOD5	SOLCOH	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	8.75E-07	8.75E-07	The correct value was returned
SOLMOD5	SOLSOH	PANEL	MS_PANEL_PABC-2009.CDB	LIBPABC-2009_PANEL	3.90E-07	3.90E-07	The correct value was returned
SULFATE	QINIT	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	6.15E+06	6.15E+06	The correct value was returned
WAS_AREA	DCELCCHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	5.10E+00	5.10E+00	The correct value was returned
WAS_AREA	DCELECHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1.34E+00	1.34E+00	The correct value was returned
WAS_AREA	DCELLCHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	4.00E+01	4.00E+01	The correct value was returned
WAS_AREA	DCELLRHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	2.20E+01	2.20E+01	The correct value was returned
WAS_AREA	DIRNCCHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1.90E+02	1.90E+02	The correct value was returned
WAS_AREA	DIRNCRHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	6.30E+02	6.30E+02	The correct value was returned
WAS_AREA	DIRONCHW	BRAGFLO	MS_BF_PABC-2009.CD	LIBPABC-2009_BF	8.10E+01	8.10E+01	The correct value was returned
WAS_AREA	DIRONRHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1.70E+02	1.70E+02	The correct value was returned
WAS_AREA	DPLASCHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	3.80E+01	3.80E+01	The correct value was returned
WAS_AREA	DPLASRHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	2.80E+01	2.80E+01	The correct value was returned
WAS_AREA	DPLSCRHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1.60E+01	1.60E+01	The correct value was returned
WAS_AREA	DPLSCRHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1.40E+01	1.40E+01	The correct value was returned
WAS_AREA	DPLSECHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	6.59E+00	6.59E+00	The correct value was returned
WAS_AREA	DRUBBCHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	5.60E+00	5.60E+00	The correct value was returned
WAS_AREA	DRUBBRHW	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	6.60E+00	6.60E+00	The correct value was returned
WAS_AREA	SMIC_CO2	BRAGFLO	MS_BF_PABC-2009.CDB	LIBPABC-2009_BF	1	1	The correct value was returned



**Table 8. Database-Code Interface Test Results for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
AM241	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	4.68E+05	4.68E+05	The correct value was returned
AM241	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	4.48E+03	4.48E+03	The correct value was returned
AM241L	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	4.85E+05	4.85E+05	The correct value was returned
AM241L	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	4.61E+03	4.61E+03	The correct value was returned
AM243	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	7.17E+01	7.17E+01	The correct value was returned
AM243	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	7.80E+00	7.80E+00	The correct value was returned
CF252	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	3.28E-02	3.28E-02	The correct value was returned
CF252	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.83E-04	1.83E-04	The correct value was returned
CM243	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.34E+00	1.34E+00	The correct value was returned
CM243	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.09E+00	2.09E+00	The correct value was returned
CM244	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.61E+03	2.61E+03	The correct value was returned
CM244	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	4.36E+02	4.36E+02	The correct value was returned
CM245	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.86E-01	5.86E-01	The correct value was returned
CM245	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	8.26E-02	8.26E-02	The correct value was returned
CM248	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.24E-01	1.24E-01	The correct value was returned
CM248	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	7.63E-03	7.63E-03	The correct value was returned
CS137	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.48E+02	5.48E+02	The correct value was returned
CS137	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	8.89E+04	8.89E+04	The correct value was returned
NP237	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	3.65E+01	3.65E+01	The correct value was returned
NP237	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.49E+00	2.49E+00	The correct value was returned
PA231	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	3.78E-01	3.78E-01	The correct value was returned

**Table 8. Database-Code Interface Test Results for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
PA231	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.87E-01	1.87E-01	The correct value was returned
PB210	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.75E+00	1.75E+00	The correct value was returned
PB210	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.43E+01	1.43E+01	The correct value was returned
PM147	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.09E-02	5.09E-02	The correct value was returned
PM147	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.18E+00	1.18E+00	The correct value was returned
PU238	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.47E+06	1.47E+06	The correct value was returned
PU238	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.11E+03	5.11E+03	The correct value was returned
PU238L	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.47E+06	1.47E+06	The correct value was returned
PU238L	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.11E+03	5.11E+03	The correct value was returned
PU239	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.10E+05	5.10E+05	The correct value was returned
PU239	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.92E+03	2.92E+03	The correct value was returned
PU239L	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	6.55E+05	6.55E+05	The correct value was returned
PU239L	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	3.92E+03	3.92E+03	The correct value was returned
PU240	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.44E+05	1.44E+05	The correct value was returned
PU240	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	9.89E+02	9.89E+02	The correct value was returned
PU241	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.06E+05	5.06E+05	The correct value was returned
PU241	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	3.94E+03	3.94E+03	The correct value was returned
PU242	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	7.46E+01	7.46E+01	The correct value was returned
PU242	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.25E+00	1.25E+00	The correct value was returned
PU244	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	3.48E-04	3.48E-04	The correct value was returned
PU244	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.34E-06	2.34E-06	The correct value was returned

**Table 8. Database-Code Interface Test Results for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
RA226	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.21E+00	2.21E+00	The correct value was returned
RA226	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.83E+01	1.83E+01	The correct value was returned
RA228	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	3.08E-01	3.08E-01	The correct value was returned
RA228	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	7.69E-02	7.69E-02	The correct value was returned
SR90	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.03E+02	5.03E+02	The correct value was returned
SR90	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	7.99E+04	7.99E+04	The correct value was returned
TH229	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	8.81E+00	8.81E+00	The correct value was returned
TH229	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	4.19E+00	4.19E+00	The correct value was returned
TH230	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.87E-01	5.87E-01	The correct value was returned
TH230	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	9.20E-03	9.20E-03	The correct value was returned
TH230L	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	9.40E+00	9.40E+00	The correct value was returned
TH230L	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	4.20E+00	4.20E+00	The correct value was returned
TH232	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.75E-01	2.75E-01	The correct value was returned
TH232	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	6.86E-02	6.86E-02	The correct value was returned
U233	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.56E+02	1.56E+02	The correct value was returned
U233	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.09E+01	5.09E+01	The correct value was returned
U234	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	3.04E+02	3.04E+02	The correct value was returned
U234	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.18E+00	5.18E+00	The correct value was returned
U234L	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	4.60E+02	4.60E+02	The correct value was returned
U234L	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	5.61E+01	5.61E+01	The correct value was returned
U235	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	4.42E+00	4.42E+00	The correct value was returned

**Table 8. Database-Code Interface Test Results for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
U235	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	7.04E-02	7.04E-02	The correct value was returned
U236	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	1.35E+00	1.35E+00	The correct value was returned
U236	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.48E-01	2.48E-01	The correct value was returned
U238	INVCHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.71E+01	2.71E+01	The correct value was returned
U238	INVRHD	PANEL	LIBPABC-2009_PANEL	LIBPABC-2009_PANEL	2.96E-01	2.96E-01	The correct value was returned
AM+3	MKD_AM	PRELHS	LHS1_PABC-2009_R2.TRN	LIBPABC-2009_LHS	Distributed	N/A	PRELHS correctly defined the proper distribution for Replicate 2
AM+3	MKD_AM	PRELHS	LHS1_PABC-2009_R3.TRN	LIBPABC-2009_LHS	Distributed	N/A	PRELHS correctly defined the proper distribution for Replicate 3
AM+3	MKD_AM	SECOTP2D	MS_ST2D_PABC-2009.CDB	LIBPABC-2009_ST2D	0.045	0.045	MATSET correctly took the median value as a placeholder
AM+3	MKD_AM	SECOTP2D	LHS3_ST2D_PABC-2009_R1_V026.CDB	LIBPABC-2009_ST2D	Distributed	0.015	Value from R1 V26. Sampled value correctly lies within sampled range of 0.005 to 0.4.
NP+4	MKD_NP	N/A	N/A	N/A	Distributed	N/A	Parameter not used in PABC-2009
NP+5	MKD_NP	N/A	N/A	N/A	Distributed	N/A	Parameter not used in PABC-2009
PU+3	MKD_PU	PRELHS	LHS1_PABC-2009_R2.TRN	LIBPABC-2009_LHS	Distributed	Distributed	PRELHS correctly defined the proper distribution for Replicate 2
PU+3	MKD_PU	PRELHS	LHS1_PABC-2009_R3.TRN	LIBPABC-2009_LHS	Distributed	Distributed	PRELHS correctly defined the proper distribution for Replicate 3
PU+3	MKD_PU	SECOTP2D	MS_ST2D_PABC-2009.CDB	LIBPABC-2009_ST2D	0.045	0.045	MATSET correctly took the median value as a placeholder
PU+3	MKD_PU	SECOTP2D	LHS3_ST2D_PABC-2009_R1_V026.CDB	LIBPABC-2009_ST2D	Distributed	0.04178	Value from R1 V26. Sampled value correctly lies within sampled range of 0.005 to 0.4.
PU+4	MKD_PU	PRELHS	LHS1_PABC-2009_R2.TRN	LIBPABC-2009_LHS	Distributed	Distributed	PRELHS correctly defined the proper distribution for Replicate 2
PU+4	MKD_PU	PRELHS	LHS1_PABC-2009_R3.TRN	LIBPABC-2009_LHS	Distributed	Distributed	PRELHS correctly defined the proper distribution for Replicate 3
PU+4	MKD_PU	SECOTP2D	MS_ST2D_PABC-2009.CDB	LIBPABC-2009_ST2D	0.071	0.071	MATSET correctly took the median value as a placeholder
PU+4	MKD_PU	SECOTP2D	LHS3_ST2D_PABC-2009_R1_V026.CDB	LIBPABC-2009_ST2D	Distributed	0.06722	Value from R1 V26. Sampled value correctly lies within sampled range of 0.0005 to 10.0.
TH+4	MKD_TH	PRELHS	LHS1_PABC-2009_R2.TRN	LIBPABC-2009_LHS	Distributed	Distributed	PRELHS correctly defined the proper distribution for Replicate 2
TH+4	MKD_TH	PRELHS	LHS1_PABC-2009_R3.TRN	LIBPABC-2009_LHS	Distributed	Distributed	PRELHS correctly defined the proper distribution for Replicate 3

**Table 8. Database-Code Interface Test Results for Parameters Used in PABC-2009 that have Changed since CRA-2009**

Material Name	Property Name	Code	File Name	Library	PAPDB Value	Value Returned	Comments
TH+4	MKD_TH	SECOTP2D	MS_ST2D_PABC-2009.CDB	LIBPABC-2009_ST2D	0.071	0.071	MATSET correctly took the median value as a placeholder
TH+4	MKD_TH	SECOTP2D	LHS3_ST2D_PABC-2009_R1_V026.CDB	LIBPABC-2009_ST2D	Distributed	0.08248	Value from R1 V26. Sampled value correctly lies within sampled range of 0.0005 to 10.0.
U+4	MKD_U	PRELHS	LHS1_PABC-2009_R2.TRN	LIBPABC-2009_LHS	Distributed	Distributed	PRELHS correctly defined the proper distribution for Replicate 2
U+4	MKD_U	PRELHS	LHS1_PABC-2009_R3.TRN	LIBPABC-2009_LHS	Distributed	Distributed	PRELHS correctly defined the proper distribution for Replicate 3
U+4	MKD_U	SECOTP2D	MS_ST2D_PABC-2009.CDB	LIBPABC-2009_ST2D	0.071	0.071	MATSET correctly took the median value as a placeholder
U+4	MKD_U	SECOTP2D	LHS3_ST2D_PABC-2009_R1_V026.CDB	LIBPABC-2009_ST2D	Distributed	0.00113	Value from R1 V26. Sampled value correctly lies within sampled range of 0.0005 to 10.0.

### 4.3 PA CODE INPUT FILE REVIEW FOR PABC-2009

During EPA's review of PABC-2004 and CRA-2009, some parameters were found to be hand-coded in the input files and not drawn from the PAPDB. Therefore, a review of the PABC-2009 PA code input files was conducted to determine if hand-coded parameters remained that, in the opinion of EPA, should have been included in the PAPDB. Using the PAPDB for this purpose is preferred, because it facilitates the traceability of parameter value changes and provides a single source for supporting documentation. Because a similar review was conducted for the CRA-2009 input files as described in Section 3.3, the PABC-2009 review focused on the changes in input files that have occurred since CRA-2009.

Models and codes used in the PABC-2009 PA are identified in Analysis Plan-145, *Analysis Plan for the CRA-2009 Performance Assessment Baseline Calculation* (Clayton 2009a [ERMS 551603]). Analysis Plan-145 also identifies new and changed parameters, as well as other changes that have occurred in the analyses since CRA-2009. Because the CRA-2009 PA calculations were based on the PABC-2004 baseline approved by EPA (EPA 2006), only those elements of the PA methodology that were potentially affected by changes since CRA-2009 were investigated. As previously mentioned, the changes since CRA-2009 include updates to the waste inventory, actinide solubilities, Culebra transmissivity fields, drilling parameters, and input files. SNL performed a comprehensive review of the PA input files between CRA-2009 and PABC-2009, and made many changes including moving hand-coded parameter values to the PAPDB. These changes added explanatory comments, moved derived material value calculations to the ALGEBRA files, and removed unused code. A QA Surveillance of the updated input files was conducted and concluded that "...overall, the defined methods for evaluating and verifying PABC-2009 Input files is satisfactorily implemented and effective in accordance with the SNL Quality implementing procedures" (Chavez 2009, Section 4.1 [ERMS 552230]).

The PABC-2009 PA calculations performed as a result of the updates from CRA-2009 involved all of the following primary codes:

- LHS - Parameter sampling
- BRAGFLO - Salado flow
- PANEL - Actinide mobilization and Salado transport
- NUTS - Salado transport
- MODFLOW - Culebra flow
- SECOTP2D – Culebra transport
- DRSPALL - Spallings releases;
- CUTTINGS\_S - Cuttings and cavings releases
- BRAGFLO\_DBR – Direct brine releases
- CCDFGF - Total release calculations
- STEPWISE - Sensitivity analysis

Inputs to three of the primary CRA-2009 PA codes, MODFLOW, SECOTP2D, and DRSPALL were not changed since PABC-2004 and the output files for these codes from PABC-2004 were

used in the CRA-2009 PA. In addition, data inputs to the PANEL code for CRA-2009 were unchanged from PABC-2004 because the waste inventory remained unchanged, and no new PANEL input files were prepared for the CRA-2009 PA. However, the updates for the PABC-2009 calculations required changes to the input files and rerunning all but the DRSPALL code. DRSPALL was therefore not rerun for PABC-2009 and the DRSPALL calculations used to generate the spillings results for the PABC-2004 PA were used in the PABC-2009 PA. STEPWISE is used as a post-processing code for sensitivity analyses of PA results and does not provide direct input to the compliance calculation. The input files for STEPWISE consist of run control parameters and output files from the primary PA codes listed above, and do not require original database parameters. It was not necessary to review the input files for codes where no changes were made.

A number of supporting codes are included as subsets of the primary codes listed above. The major supporting codes that require data inputs not derived from other PA codes include SANTOS (repository porosity), FMT (actinide solubility), GENMESH (mesh generation), MATSET (parameter identification and values), ICSET (initial conditions), ALGEBRA (derived properties), PREBRAG (input files for BRAGFLO), PRELHS (sampled parameter values), and EPAUNI (inventory activities).

No new SANTOS calculations have been conducted since the CCA; therefore, SANTOS output files from the CCA were used in both CRA-2009 and PABC-2009. The FMT code was used to recalculate actinide solubilities based on updated data and provide those results to PANEL. While not directly used in the PA release calculations, the FMT input and output files were reviewed by EPA as part of its assessment of the WIPP actinide chemistry. Although EPAUNI was not rerun for CRA-2009, it was rerun for PABC-2009 because of the updated waste inventory and the updated input files for EPAUNI were reviewed by EPA. As described more fully in Section 3.3, the MATSET code provides input values for the constant parameters and placeholder values for the distributed parameters, and the LHS code subsequently replaces the placeholder values with the sampled values used in PA.

This review was conducted by comparing the input files for each of the primary codes identified above that were changed since CRA-2009. Changes in input files were identified using the *difference* command in the VMS operating system. Numerical inputs that were not drawn from the PAPDB, but were hand-coded into the input files, were identified visually and are documented in the following sections. Additional information can be found in the user's manuals for the various codes.

#### **4.3.1 BRAGFLO Assessment**

BRAGFLO is a two-phase flow code that simulates brine and gas flow in and around the WIPP repository, and incorporates the effects of disposal room closure, gas generation, brine consumption, and inter-bed fracturing in response to gas pressure (Clayton 2008a, Section 2.6.2 [ERMS 547905]). The following BRAGFLO input files were compared:

GENMESH Input Files:       GM\_BF\_PABC-2009.INP compared with GM\_BF\_CRA-2009.INP

MATSET Input Files: MS\_BF\_PABC-2009.INP compared with MS\_BF\_CRA-2009.INP  
ICSET Input Files: IC\_BF\_PABC-2009.INP compared with IC\_BF\_CRA-2009.INP  
ALGEBRA Input Files: ALG1\_BF\_PABC-2009.INP compared with ALG1\_BF\_CRA-  
2009.INP  
ALG2\_BF\_PABC-2009.INP compared with ALG2\_BF\_CRA-  
2009.INP  
PREBRAG Input Files: BF1\_PABC-2009\_S1.INP compared with BF1\_CRA-  
2009\_S1.INP  
BF1\_PABC-2009\_S2.INP compared with BF1\_CRA-  
2009\_S2.INP

**The GENMESH input file** defines the computational grid framework for the BRAGFLO analyses. No hand-coded parameter values were found in the PABC-2009 difference file.

**The MATSET input files** for BRAGFLO provides parameter values for the BRAGFLO analyses. Previously hand-coded parameters have been removed from the input file and the values for these parameters are now drawn from the PAPDB. No remaining hand-coded parameter values were found in the PABC-2009 difference file.

**The ICSET input file** establishes initial conditions for the BRAGFLO analyses. No hand-coded parameter values were found in the PABC-2009 difference file.

**Two ALGEBRA files** are used by BRAGFLO. ALGEBRA1 computes derived properties for BRAGFLO that cannot be obtained from the PAPDB. ALGEBRA2 is a post-processor for the results of the BRAGFLO calculations.

Excluding unit conversion factors, the following hand-coded parameter values remain in the PABC-2009 **ALGEBRA1** input file for BRAGFLO:

Code Lines 154, 322 & 711:  $SB\_MIN = 1.05 * SAT\_RBRN$

The factor 1.05 is used to calculate minimum brine saturation when using capillary pressure Model 3; otherwise, this factor is not used. This factor was also present in the ALGEBRA1 file for PABC-2004, and was identified in EPA's PABC-2004 parameter review, with the recommendation that it be added to the PAPDB. Although EPA continued to recommend drawing this factor from the PAPDB in its CRA-2009 review, additional analysis during the PABC-2009 review confirmed that this factor is not currently used in PA and that documentation in the BRAGFLO User's Manual provides adequate traceability (Nemer 2006, p. 135 [ERMS 545016]). EPA therefore concludes that this factor need not be entered into the PAPDB.

The following hand-coded parameter values remain in the PABC-2009 **ALGEBRA2** input file for BRAGFLO:



Code Line 728:  $BRN\_RMV = -1.0 * BRN\_CON / DNSFLUID[B:26]$   
The factor -1.0 is inserted to make BRN\_RMV a negative value. This factor is repeated in many subsequent code lines. EPA considers these to be run control parameters.

**The PREBRAG code** prepares input files in a format compatible for BRAGFLO. Separate input files are prepared for Scenario 1 (the undisturbed scenario where no drilling intrusion occurs) and Scenarios 2 through 6 (disturbed scenarios where one or more drilling intrusions occur). The input files for Scenarios 2 through 6 use the same types of numerical inputs, and the files for Scenarios 1 and 2 were selected by EPA for this review.

Previously hand-coded parameters have been removed from the PREBRAG input files for both Scenarios 1 and 2, and the values for these parameters are now drawn from the PAPDB. No remaining hand-coded parameter values were found in the PABC-2009 input difference files for either scenario.

### 4.3.2 BRAGFLO\_DBR Assessment

The BRAGFLO code is run in the Direct Brine Release (DBR) mode to calculate brine releases from a pressurized repository through an intruding borehole (Clayton 2008a, Section 2.6.7 [ERMS 547905]). The following BRAGFLO\_DBR input files were compared:

GENMESH Input Files:	GM_DBR_PABC-2009.INP compared with GM_DBR_CRA-2009.INP
MATSET Input Files:	MS_DBR_PABC-2009.INP compared with MS_DBR_CRA-2009.INP
ICSET Input Files:	IC_DBR_PABC-2009_S1.INP compared with IC_DBR_CRA-2009_S1.INP IC_DBR_PABC-2009_S2.INP compared with IC_DBR_CRA-2009_S2.INP
ALGEBRA Input Files:	ALG1_DBR_PABC-2009.INP compared with ALG1_DBR_CRA-2009.INP ALG2_DBR_PABC-2009_S1.INP compared with ALG2_DBR_CRA-2009_S1.INP ALG2_DBR_PABC-2009_S2.INP compared with ALG2_DBR_CRA-2009_S2.INP ALG3_DBR_PABC-2009.INP compared with ALG3_DBR_CRA-2009.INP
RELATE Input Files:	REL1_DBR_PABC-2009.INP compared with REL1_DBR_CRA-2009.INP REL2_DBR_PABC-2009_S1.INP compared with REL2_DBR_CRA-2009_S1.INP

REL2\_DBR\_PABC-2009\_S2.INP compared with  
REL2\_DBR\_CRA-2009\_S2.INP

PREBRAG Input Files: BF1\_DBR\_PABC-2009\_L.INP compared with BF1\_DBR\_CRA-  
2009\_S1\_L.INP  
BF1\_DBR\_PABC-2009\_M.INP compared with BF1\_DBR\_CRA-  
2009\_S1\_M.INP  
BF1\_DBR\_PABC-2009\_U.INP compared with BF1\_DBR\_CRA-  
2009\_S1\_U.INP  
BF1\_DBR\_PABC-2009\_L.INP compared with BF1\_DBR\_CRA-  
2009\_S2\_L.INP  
BF1\_DBR\_PABC-2009\_M.INP compared with BF1\_DBR\_CRA-  
2009\_S2\_M.INP  
BF1\_DBR\_PABC-2009\_U.INP compared with BF1\_DBR\_CRA-  
2009\_S2\_U.INP

**The GENMESH input file** defines the computational grid framework for the BRAGFLO\_DBR analyses. The following hand-coded parameter values remain in the PABC-2009 GENMESH input file for BRAGFLO\_DBR:

Code Lines 93 to 96: DEL, COORD = Y, DEL = 30.50, INRANGE = 4,5, FACTOR = 1  
DEL, COORD = Y, DEL = 30.50, INRANGE = 5,6, FACTOR = 1  
DEL, COORD = Y, DEL = 30.50, INRANGE = 6,7, FACTOR = 1  
DEL, COORD = Y, DEL = 4.30, INRANGE = 7,8, FACTOR = 1

These hand-coded values modify the BRAGFLO\_DBR grid in the y-dimension to make the volume of the panels in BRAGFLO\_DBR the same as the volume of the representative panel in BRAGFLO. EPA considers these to be run control parameters.

**The MATSET input files** for BRAGFLO\_DBR provide parameter values for the BRAGFLO\_DBR analyses. No hand-coded parameter values were found in the PABC-2009 difference file.

**The ICSET input file** establishes initial conditions for the BRAGFLO\_DBR analyses. Separate input files are prepared for Scenario 1 (the undisturbed scenario where no drilling intrusion occurs) and Scenarios 2 through 5 (disturbed scenarios where one drilling intrusion occurs). Five drilling scenarios are used instead of six in this and some subsequent analyses, because Scenario 6 is used to model long-term releases from multiple intrusions. BRAGFLO\_DBR is used to model short-term releases from single intrusions, which only involve Scenarios 1 through 5. The input files for Scenarios 2 through 5 use the same types of numerical inputs, and the file for Scenario 2 was selected by EPA for this review.

The ICSET input files for BRAGFLO\_DBR Scenarios 1 and 2 were reviewed by EPA and no hand-coded parameter values were found in the PABC-2009 difference file.

**The ALGEBRA files** compute derived properties that cannot be obtained from the PAPDB. There are three different types of ALGEBRA files for BRAGFLO\_DBR. ALGEBRA1 is used







NUTS SCN Input Files: NUT\_SCN\_PABC-2009\_S1.INP compared with  
NUT\_SCN\_CRA-2009\_S1.INP  
NUT\_SCN\_PABC-2009\_S2.INP compared with  
NUT\_SCN\_CRA-2009\_S2.INP

ALGEBRA SCN Input Files: ALG\_NUT\_SCN\_PABC-2009.INP compared with  
ALG\_NUT\_SCN\_CRA-2009.INP

MATSET Input Files: New File

NUTS ISO Input Files: NUT\_ISO\_PABC-2009\_S1.INP compared with NUT\_ISO\_CRA-  
2009\_S1.INP  
NUT\_ISO\_PABC-2009\_S2.INP compared with NUT\_ISO\_CRA-  
2009\_S2.INP

ALGEBRA ISO Input Files: ALG\_NUT\_ISO\_PABC-2009.INP compared with  
ALG\_NUT\_ISO\_CRA-2009\_S1.INP  
ALG\_NUT\_ISO\_PABC-2009.INP compared with  
ALG\_NUT\_ISO\_CRA-2009\_S2.INP

NUTS INT Input Files: NUT\_INT\_PABC-2009\_S2\_T00100.INP compared with  
NUT\_INT\_CRA-2009\_S2\_T00100.INP

ALGEBRA INT Input Files: Uses the ALGEBRA ISO input files (see below)

**The NUTS SCN code** provides a screening analysis to identify vector-scenario combinations that warrant a full transport analysis. NUTS SCN input files are scenario specific. As before, separate input files are prepared for Scenario 1 (the undisturbed scenario where no drilling intrusion occurs) and Scenarios 2 through 5 (disturbed scenarios where one drilling intrusion occurs). The NUTS SCN input files for Scenarios 2 through 5 use the same types of numerical inputs, and the input files for Scenarios 1 and 2 were selected by EPA for this review. No hand-coded parameter values were found in either of these PABC-2009 difference files.

**The NUTS ALGEBRA SCN code** post-processes the NUTS SCN screening run outputs. The ALGEBRA SCN input files are not scenario specific. No hand-coded parameter values were found in the PABC-2009 input difference file.

**The NUTS MATSET code** is a new code for PABC-2009 structured to draw radionuclide isotope input parameters from the PAPDB. No hand-coded parameter values were found in this PABC-2009 file.

**The NUTS ISO code** calculates radionuclide transport through the Salado to the land withdrawal boundary, and transport through an intrusion borehole and shaft to the Culebra. The NUTS ISO input files are scenario specific, as described above for the NUTS SCN code. The NUTS ISO input files for Scenarios 1 and 2 were selected by EPA for this review. No hand-coded parameter values were found in either of these PABC-2009 difference files.

**The NUTS ALGEBRA ISO code** post-processes the NUTS ISO outputs. Although separate input files were previously required for each drilling scenario, the input files were modified for PABC-2009 to be independent of drilling scenario and only one NUTS ALGEBRA ISO input file is now needed. As a check on the accuracy of this input file revision, EPA compared the PABC-2009 input file with the CRA-2009 input files for drilling Scenarios 1 and 2. With the exception of unit conversion factors, no hand-coded parameter values were found in either of these PABC-2009 difference files.

**The NUTS INT code** calculates radionuclide transport through an intrusion borehole and shaft to the Culebra for intrusion times other than the 350- and 1000-year intrusion times modeled in BRAGFLO. The example selected by EPA for review models radionuclide transport for a Scenario 2 borehole intrusion at 100 years that intersects a Castile brine pocket. No hand-coded parameter values were found in this PABC-2009 file.

**The NUTS ALGEBRA INT code** post-processes the NUTS INT outputs. The requirements for this code are the same as the ALGEBRA ISO code and the ALGEBRA ISO code is used in PA.

#### **4.3.5 PANEL Assessment**

The PANEL code is used to calculate radionuclide transport to the Culebra for drilling Scenario S6. This scenario assumes the repository is intersected by two boreholes, one where an underlying brine pocket is hit and another where a brine pocket is not hit. PANEL was not run in the CRA-2009 PA because the inventory was unchanged from the previous PABC-2004 PA. PANEL input files for PABC-2009 were therefore compared with the input files for PABC-2004. As was previously noted, PABC-2004 is identified as CRA1BC in the input files. The previous ALGEBRA input file for PANEL (ALG\_PANEL\_CRA1BC.INP) included a sub-calculation called ALG\_MOLE.INP. During SNL's input file review for PABC-2009, the ALGEBRA input file for PANEL was split into two files (ALGEBRA1, consisting of the former input file ALG\_MOLE.INP; and ALGEBRA3, consisting of the former input file ALG\_PANEL\_CRA1BC.INP). In addition, a new ALGEBRA2 input file was created to perform calculations that were formerly performed outside the PA models. The following PANEL input files used in PABC-2009 were compared:

GENMESH Input Files: GM\_PANEL\_PABC-2009.INP compared with  
GM\_PANEL\_CRA1BC.INP

MATSET Input Files: MS\_PANEL\_PABC-2009.INP compared with  
MS\_PANEL\_CRA1BC.INP

ALGEBRA1 Input Files: ALG1\_PANEL\_PABC-2009.INP compared with  
ALG\_MOLE.INP

ALGEBRA2 Input Files: ALG2\_PANEL\_PABC-2009.INP – newly created for PABC-2009

ALGEBRA3 Input Files: ALG3\_PANEL\_PABC-2009.INP compared with  
ALG\_PANEL\_CRA1BC.INP

**The GENMESH input file** defines the computational grid framework for the PANEL analyses. No hand-coded parameter values were found in the PABC-2009 input difference file.

**The MATSET input file** provides parameter values for the PANEL analyses. No hand-coded parameter values were found in the PABC-2009 input difference file.

**The ALGEBRA1 input file** is used to calculate the total moles of U, Pu, and Th, and the mole fractions of U233+U234, PU238, and TH229+PU230. This was previously a separate file called ALG\_MOLE.INP that supported the original PANEL ALGEBRA input file. No hand-coded parameter values were found in the PABC-2009 input difference file.

**The ALGEBRA2 input file** is used to set the maximum over time of the Log Sol difference. No hand-coded parameter values were found in the PABC-2009 input difference file.

**The ALGEBRA3 input file** is the new name for the previous PANEL input file ALG\_PANEL\_CRA1BC.INP. No hand-coded parameter values were found in the PABC-2009 input difference file.

#### **4.3.6 MODFLOW Assessment**

The MODFLOW code is used to calculate groundwater flow fields in the Culebra. MODFLOW was run in PABC-2009 because of changes made to the Culebra T-fields since CRA-2009. MODFLOW was originally developed by the U.S. Geological Survey and was not written to draw input parameter values from the PAPDB. Instead, SNL uses the following file transfer steps:

First, the PA code SECOTP2D (described below) is used to provide the following input information to MODFLOW using File Transfer Protocol (FTP) to transfer data as text files from the VMS system used in PA to the LINUX system used by MODFLOW:

- 1) The mining modification factor CULEBRA:MINP\_FAC
- 2) The climate modification factor GLOBAL:CLIMTIDX
- 3) Indices for mapping transmissivity fields to individual vectors  
GLOBAL:TRANSIDX

Second, MODFLOW is used to calculate the Culebra flow fields using the foregoing inputs from SECOTP2D and the following inputs from the CVS repository library in LINUX:

- 1) One hundred calibrated, unmodified T-fields and grid dimensions
- 2) Utility scripts providing directions for applying the mining factors to the unmodified T-fields to calculate Culebra flow fields.

Third, the calculated MODFLOW flow fields are transferred back to the VMS system as FTP flow field arrays, which are used by SECOTP2D to calculate radionuclide transport in the Culebra.

The MODFLOW run controls for the PABC-2009 PA are provided in the file MINING\_MOD.INP. This file identifies the libraries where the calibrated T-fields, mining





MATSET Input Files: MS\_ST2D\_PABC-2009.INP compared with MS\_ST2D\_CRA1BC.INP

ALGEBRA Input Files: ALG\_ST2D\_PABC-2009.INP compared with ALG\_ST2D\_CRA1BC.INP

RELATE Input Files: REL\_ST2D\_PABC-2009.INP compared with REL\_ST2D\_CRA1BC.INP

VTRAN2 Input Files: VTRAN2\_PABC-2009.INP compared with VTRAN2\_CRA1BC.INP

PRESECOTP2D Input Files: ST2D1\_PABC-2009.INP compared with ST2D1\_CRA1BC.INP

**The GENMESH input file** defines the computational grid framework for the SECOTP2D analyses. No hand-coded parameter values were found in the PABC-2009 input difference file.

**The MATSET input file** provides parameter values for the SECOTP2D analyses. No hand-coded parameter values were found in the PABC-2009 input difference file.

The **ALGEBRA input file** is used to perform internal calculations for the SECOTP2D analyses. A previously hand entered activity constant was removed from the input file and is now calculated using Avogadro's number and a unit conversion factor, both drawn from the PAPDB. No hand-coded parameter values were found in the PABC-2009 input difference file.

The **RELATE input file** provides SECOTP2D with the values of calculated properties and sampled parameters developed by other codes. This file is unchanged from PABC-2004 and no hand-coded parameter values were therefore found in the PABC-2009 input difference file.

The **VTRAN2 input file** converts output from MODFLOW to input for SECOTP2D. The following hand-coded parameter values remain in the PABC-2009 VTRAN2 input file for SECOTP2D:

Code Line 8: (568e24.16)

This code line specifies the input format: the number of grid cells (568) in the x-direction (east to west), the number of digits (24), and the number of places after the decimal (16), indicating a double precision calculation. EPA does not consider these run control parameters to be database values.

Code Line 12: 568 614

This code line specifies the number of grid cells: 568 in the x-direction and 614 in the y-direction. EPA does not consider these run control parameters to be database values.

The **PRESECOTO2D input file** prepares input files in a format compatible for SECOTP2D. This file is unchanged from PABC-2004 and no hand-coded parameter values were therefore found in the PABC-2009 input difference file.

#### 4.3.8 EPAUNI Assessment

The EPAUNI code is used to convert estimated releases from the WIPP repository to normalized values called EPA units. EPA units are calculated as the estimated release of a radionuclide divided by the EPA release limit for that radionuclide and by the waste unit factor (BOREHOLE:WUF). For PABC-2009, EPA units are calculated for alpha-emitting transuranic radionuclides with half lives greater than 20 years, decayed to the year 2033. These values were previously decayed to the year 2001 in PABC-2004. EPAUNI was not run in the CRA-2009 PA because the waste inventory was unchanged from PABC-2004. EPAUNI input files are not designed to draw parameter values from the PAPDB nor are they configured with comments. EPAUNI input files for PABC-2009 were comprehensively updated from PABC-2004 and were reviewed in their entirety. The following files provided inputs to EPAUNI for PABC-2009:

MISCELLANEOUS Input Files:   EPU\_PABC-2009\_CH\_MISC.INP  
                                  EPU\_PABC-2009\_RH\_MISC.INP  
EPAUNI Input Files:         EPU\_PABC-2009\_CH.INP  
                                  EPU\_PABC-2009\_RH.INP

The two **MISCELLANEOUS input files** for EPAUNI address contact handled and remote handled waste. The MISCELLANEOUS files provide run control parameters for EPAUNI that are identical for the two types of waste. The entire MISCELLANEOUS input file for both waste types, consisting of two lines, is reproduced below.

```
0 2 0 0 2033
2.60
```

The sequence 0 2 0 0 in the first line provides run controls for input files to be read and output files to be produced. The number 2033 in the first line indicates the year to which the waste is decayed. The number 2.60 in the second line is the value of the waste unit factor for PABC-2009, which has been entered into the PAPDB as the parameter BOREHOLE:WUF.

The two EPAUNI input files provide the total waste volume and the activities in Curies of the 10 radionuclides used to calculate EPA units, for each WIPP waste stream. For PABC-2009, there are 405 CH waste streams and 70 RH waste streams, with a combined total of  $(475 \times 11 =) 5,225$  parameter values. These two input files are uncommented but provide headers identifying the parameter type in each column of the array. The EPAUNI input files are automatically generated from the electronic records and that the input file records are documented electronically in the SNL Records Center on a disc attached to Fox et al. 2009 [ERMS 551679]. In addition, hard copies of the input files are provided in Clayton 2010, Tables 39 and 40 [ERMS 552889].

In response to EPA's observation that there is a lack of traceability between the input files and the data sources, SNL agreed to enter comments into the MISCELLANEOUS input files describing those data sources. Comments cannot be entered into the EPAUNI input files because they are limited to the file structure specified in the EPAUNI code. In addition, EPA checked the input requirements documentation in the EPAUNI User's Manuals (Leigh 2003 [ERMS

529570] and Trone 2003 [ERMS 530203]) and found it to be adequate. EPA considers the addition of source document information into the MISCELLANEOUS input files to adequately provide the needed traceability for EPAUNI input data because such information would be readily identified from either a comprehensive review of the input files or a review of the user's manuals.

#### 4.3.9 CCDFGF Assessment

The CCDFGF code is used to assemble calculated release data from various PA codes into complementary cumulative distribution functions (CCDFs) for comparison with regulatory release limits. EPAUNI is a preprocessor for CCDFGF and is individually assessed in Section 4.3.8. The following CCDFGF input files used in PABC-2009 were compared with those used in CRA-2009:

GENMESH Input Files: GM\_CCGF\_PABC-2009.INP compared with GM\_CCGF\_CRA-2009.INP

MATSET Input Files: MS\_CCGF\_PABC-2009.INP compared with MS\_CCGF\_CRA-2009.INP

CONTROL Input Files: CCGF\_PABC-2009\_CONTROL\_R1.INP compared with CCGF\_CRA-2009\_CONTROL\_R1.INP

**The GENMESH input file** defines the single cell mesh used in the CCDFGF calculation. No hand-coded parameter values were found in the PABC-2009 input difference file.

**The MATSET input file** provides parameter values for the CCDFGF analyses. No hand-coded parameter values were found in the PABC-2009 input difference file.

**The CONTROL input file** contains CCDFGF run control data. The CONTROL input files for the three replicates calculated in PA are essentially the same. The input file for Replicate 1 was selected by EPA for review. No hand-coded parameter values were found in the PABC-2009 input difference file.

#### 4.3.10 PRELHS Assessment

As previously explained the PRELHS code takes distribution information for all sampled parameters from the PAPDB and provides the information to the LHS code, which selects 100 sampled values for each distributed parameter. One set of these sampled values is used in each realization. Because PRELHS takes distribution information for all sampled parameters and is not specific to a given primary code, the PRELHS input files are replicate specific. All three replicates were reviewed by EPA. The following PRELHS input files were compared:

PRELHS Input Files: LHS1\_PABC-2009\_R1.INP compared with LHS1\_CRA-2009\_R1.INP

LHS1\_PABC-2009\_R2.INP compared with LHS1\_CRA-2009\_R2.INP

LHS1\_PABC-2009\_R3.INP compared with LHS1\_CRA-2009\_R3.INP

The hand-coded parameter NOBS 100 was identified in Code Lines 23 and 35 of the PRELHS PABC-2009 input files for all three replicates. These entries identify the number of samples of an uncertain parameter in a replicate. The same entries were made in the PRELHS input files for CRA-2009. EPA continues to consider NOBS 100 to be a run control parameter. No other hand-coded parameter values were found in the PABC-2009 input difference file.

#### **4.3.11 Summary of PABC-2009 Input File Review**

The focus of EPA's review of the PABC-2009 input files was on changes that occurred since CRA-2009. All identified changes involving hand-coded numerical inputs were found to be run control rather than database parameters. The input files for two codes, MODFLOW and EPAUNI, were not designed to draw parameter values from the PAPDB. The PABC-2009 run controls for MODFLOW are provided in the files MINING\_MOD.INP and KEEPERS. Although the file MINING\_MOD.INP is extensively commented and refers to KEEPERS as a supporting file, EPA observed that the comments did not explicitly identify the file as applicable to the PABC-2009 PA, nor did the comments provide traceability to the source documentation for the input parameters. SNL agreed to add comments to MINING\_MOD.INP addressing these observations. The PABC-2009 input files for EPAUNI, called MISCELLANEOUS and EPAUNI, were found to be uncommented and thus provided no traceability to either PABC-2009 or to the source documentation for the input parameters. SNL demonstrated that the MISCELLANEOUS input file could be commented, while the EPAUNI input file could not. SNL agreed to add comments to the MISCELLANEOUS input file providing traceability to PABC-2009, to the EPAUNI input file, and to the source documentation for the input parameters. In addition, EPA found that the EPAUNI User's Manual provided adequate traceability for both input files. In consideration of the input file modifications agreed upon by SNL, EPA considers the traceability of the input files for MODFLOW and EPAUNI to be adequate.

## **5.0 STATUS OF PRIOR EPA RECOMMENDATIONS FOR HAND-CODED PARAMETERS**

As part of EPA's review of PABC-2004 input files, several recommendations were made for transferring hand-coded parameters to the PAPDB. As previously discussed, the primary reason for transferring parameters to the PAPDB was to improve traceability. These recommendations were reviewed with Dan Clayton of SNL during the PABC-2009 review to determine their current status. These recommendations and their current status are summarized in Table 9.

Many of EPA's recommendations were acted upon by DOE and the hand-coded values were removed from the input files and added to the PAPDB. During the PABC-2009 review, EPA reevaluated those parameters that DOE considered to be numerical code controls with emphasis on their use, traceability, physical basis, likelihood to change, and primary purpose. EPA concluded that numerical values that were clearly used for run control by virtue of the coding structure of the input files were not parameters and should not be entered into the database. An example of this is a numerical value that identifies a specific grid block location. Numerical values whose purpose was less clearly evident should be traceable to an explanation of purpose and basis. This traceability should be readily identifiable through documentation in logical places such as comments within the input files themselves or in the user's manual for the code. Numerical inputs that have a physical basis but are highly unlikely to change, such as unit conversion factors, can appropriately be hand-coded. Numerical inputs that stabilize or delimit a computational process fall into a gray area between numerical control and database parameters. To be considered numerical control parameters they should, as a minimum, have the primary purpose of controlling numerical processes and be readily traceable to an explanation of purpose and basis. Examples are parameters set to small minimum values to avoid model instabilities, parameters that allow time for initiation of transients, and parameters that eliminate round-off errors in very small numbers. EPA accepts that such parameters can be considered numerical control parameters if they are readily traceable, such as clearly explained in the code's User's Manual, and has applied these criteria when developing the conclusory observations in Table 9.

EPA has also observed that DOE occasionally considers hand-coded input parameters that are not used in PA calculations to be numerical control parameters even though they would otherwise be considered database parameters. An example relevant to Table 9 is the parameter SPALLMOD:MAXPRESS, which establishes the maximum pressure for the mud pump in a drilling operation for the DRSPALL model. A value of 27.5 MPa was selected from literature from oilfield mud pump manufacturers. However, this parameter was not used by the DRSPALL code because the drill pipe portion of the model was turned off and a constant mud flow rate was instead imposed at the drill bit. Parameters such as this that are not used do not require the traceability of parameters that are used; however, if and when such parameters are used, they should be entered into the PAPDB where traceability is procedurally provided.

**Table 9. Status of Prior EPA Recommendations for Hard-Coded Parameters**

<b>Code</b>	<b>Parameter</b>	<b>Parameter Type</b>	<b>DOE Response</b>	<b>EPA Observation</b>
DRSPALL	SPALLMOD:CHARLEN	Characteristic length for tensile failure	Numerical control parameter not suitable for entry into the PAPDB	Response accepted. Traceability is established in the DRSPALL input files DRS*.INP.
DRSPALL	SPALLMOD:DRZTCK	DRZ thickness	Added to PAPDB as new parameter SPALLMOD:DRZTCK	Response accepted. Traceability is established through the PAPDB.
DRSPALL	SPALLMOD:INITBAR	Initial height above the repository	Numerical control parameter not suitable for entry into the PAPDB	Response accepted. Traceability is established in the DRSPALL input files DRS*.INP.
DRSPALL	SPALLMOD:EXITPLEN	Exit pipe length	Numerical control parameter not suitable for entry into the PAPDB	Response accepted. Traceability is established in the DRSPALL input files DRS*.INP.
DRSPALL	SPALLMOD:EXITPDIA	Exit pipe diameter	Numerical control parameter not suitable for entry into the PAPDB	Response accepted. Traceability is established in the DRSPALL input files DRS*.INP.
DRSPALL	SPALLMOD:FRCHBETA	Frochheimer Beta	Added to PAPDB as new parameter SPALLMOD:FRCHBETA	Response accepted. Traceability is established through the PAPDB.
DRSPALL	SPALLMOD:MAXPPRES	Maximum mud pump pressure	Numerical control parameter not suitable for entry into the PAPDB	Response accepted. Traceability is established in the DRSPALL input files DRS*.INP.
DRSPALL	SPALLMOD:REPOSTCK	Repository thickness	Added to PAPDB as new parameter SPALLMOD:REPOSTCK	Response accepted. Traceability is established through the PAPDB.
DRSPALL	SPALLMOD:REPOTRAD	Repository domain outer radius	Added to PAPDB as new parameter SPALLMOD:REPOTRAD	Response accepted. Traceability is established through the PAPDB.
DRSPALL	SPALLMOD:STPDTIME	Stop drilling time	Numerical control parameter not suitable for entry into the PAPDB	Response accepted. Traceability is established in the DRSPALL input files DRS*.INP.
BRAGFLO	DRF_PCS:*	Properties of the panel closure system drifts	Derived material set equal to the equivalent WAS_AREA properties	Response rejected. Traceability lacking. Dan Clayton of SNL agreed to add this material and its properties to the PAPDB.
BRAGFLO / DBR	DIP1	Repository dip angle	Added to PAPDB as new parameter REFCON:DIP1	Response accepted. Traceability is established through the PAPDB.
BRAGFLO	DIP2	Rustler formation dip angle	Added to PAPDB as new parameter REFCON:DIP2	Response accepted. Traceability is established through the PAPDB.
BRAGFLO	1.05	Minimum brine saturation factor	Numerical control parameter not suitable for entry into the PAPDB	Response accepted. See Section 3.3.7 and Table 4.

**Table 9. Status of Prior EPA Recommendations for Hard-Coded Parameters**

<b>Code</b>	<b>Parameter</b>	<b>Parameter Type</b>	<b>DOE Response</b>	<b>EPA Observation</b>
DBR	WAS_AREA:HEIGHT WAS_AREA:*SPAN1 WAS_AREA:*SPAN2 WAS_AREA:*SPAN3	Height, brine and gas pressures and saturations for drilling locations 1, 2, and 3	Derived materials with values based on post-processed BRAGFLO and CUTTINGS_S results. Gas pressure and saturation parameters are not used in PA and were removed. For remaining parameters, the input files were revised to set values in RELATE instead of overriding a dummy values set in MATSET.	Response accepted. Traceability provided by parameter value transfer information in the RELATE input file.
DBR	DRZ_CONC:*	Properties of the DRZ next to the panel closure concrete	Derived materials set equal to the equivalent DRZ_1 properties or to a combination of DRZ_1 and CONC_PCS properties	Response rejected. Traceability lacking. Dan Clayton of SNL agreed to add explanatory comments to relevant input files.
DBR	PAN_SL2:*	Properties of middle panel closures with a different orientation than standard panel closures	Derived materials with revised directional properties and remaining properties set equal to the equivalent CONC_PCS properties	Response rejected. Traceability lacking. Dan Clayton of SNL agreed to add explanatory comments to relevant input files.
DBR	WELLBORE:*	Properties of intrusion well	Derived materials. Files revised to set all values in ALGEBRA instead of some in ALGEBRA and some in MATSET. Values based on post-processed CUTTINGS_S results.	Response accepted. Setting all values in commented ALGEBRA file is sufficient to explicitly identify these parameters as calculated values.
DBR	DRZ_1:HEIGHT	Effective height of the DRZ	Added to PAPDB as new parameter DRZ_1:EHEIGHT	Response accepted. Traceability is established through the PAPDB.
DBR	DRZ_1:PERMBRX	Permeability of the DRZ at time of intrusion	Derived material. Files revised to set value in ALGEBRA instead of MATSET. Values based on post-processed CUTTINGS_S results.	Response accepted. Setting value in commented ALGEBRA file is sufficient to explicitly identify this parameter as a calculated value.
DBR	DRZ_1:POR_INTR	Porosity of the DRZ at time of intrusion	Derived material. Files revised to set value in ALGEBRA instead of MATSET. Values based on post-processed CUTTINGS_S results.	Response accepted. Setting value in commented ALGEBRA file is sufficient to explicitly identify this parameter as a calculated value.
DBR	S_HALITE:HEIGHT	Effective height of the halite pillars between rooms in a waste panel	Parameter not used and was deleted	Response accepted.



**Table 9. Status of Prior EPA Recommendations for Hard-Coded Parameters**

<b>Code</b>	<b>Parameter</b>	<b>Parameter Type</b>	<b>DOE Response</b>	<b>EPA Observation</b>
BRAGFLO / DBR	REFCON:DIP_DEG	Repository dip angle	Added to PAPDB as new parameter REFCON:DIP1	Response accepted. Traceability is established through the PAPDB.
DBR	D1	Thickness of panel closure empty drift and explosion wall	Added to PAPDB as new parameter CONC_PCS:THKOPEN	Response accepted. Traceability is established through the PAPDB.
DBR	D2	Thickness of panel closure concrete	Added to PAPDB as new parameter CONC_PCS:THKCONC	Response accepted. Traceability is established through the PAPDB.
DBR	DE	Total thickness of panel closure drift	Replaced by sum of CONC_PCS:THKOPEN and CONC_PCS:THKCONC	Response accepted. Traceability is established through the PAPDB.
DBR	FBHP	Flowing bottom hole pressure	Derived material value calculated in ALGEBRA	Response accepted. Setting value in commented ALGEBRA file is sufficient to explicitly identify this parameter as a calculated value.
DBR	H2_MOLE CO2_MOLE CH4_MOLE N2_MOLE H2S_MOLE O2_MOLE	Flags given 0 or 1 values identifying the gas used to represent the gas generated in the repository	Run control parameters	Response accepted. These parameters are defined in the PREBRAG Users Manual (Gilkey and Rudeen 2007, ERMS 545274)

## 6.0 PARAMETER DATA ENTRY PROCESS REVIEW

Parameter data entry process and control were evaluated by reviewing the PDE forms used as the basis for data entry into the PAPDB, in accordance with SNL Procedure NP 9-2 Rev 01, *Parameters*. This procedure was most recently updated in August 2006. It prescribes the processes for developing, documenting, controlling, and changing parameters used in compliance-level and programmatic PA calculations performed by SNL in support of the WIPP. Parameter values are required to be developed and documented in accordance with approved, procedurally driven planning documents. NP 9-2 Rev 01 provides detailed instructions for entering or changing a parameter value in the PAPDB. Responsibilities for checking and approval are clearly defined and appropriate. No concerns regarding this procedure were identified in this review.

EPA also reviewed Activity Specific Procedure SP 9-5 Rev 01, *Parameter Data Entry*. This procedure was most recently updated in October 2006. It establishes the process for entering or editing parameter information in the PAPDB and is intended to ensure that parameter information is entered correctly. The procedure provides specific instructions for creating a parameter, creating an analysis, creating computational codes, entering parameter values, replacing parameter values, and creating justification documentation. EPA found this procedure to be comprehensive and appropriate. No concerns regarding this procedure were identified in this review.

Each PDE form for the 255 parameters that are new or have been changed since PABC-2004 was inspected for completeness to confirm that all appropriate blanks were filled in and the necessary signatures were provided. Accuracy of the data entry process was checked by visually comparing the information on the form with the information shown in the online PAPDB. In no cases were errors found in the entered parameter values when compared to the forms.

A review of the PDE forms supporting the parameter changes between PABC-2004 and CRA-2009 determined that they were completely and correctly filled out. Handwritten changes were found on two of the forms (the forms for parameters DRZ\_0:POROSITY [ERMS 545794] and DRZ\_1:POROSITY [ERMS 545795]), correcting the identification number of the associated Analysis Plan. These hand entries were dated and initialed by the originator of the form and were, therefore, acceptable.

A review of the PDE forms supporting the parameter changes between CRA-2009 and PABC-2009 found one error: the supporting documentation attached to the PDE for parameter BOREHOLE:WUF [ERMS 552242] incorrectly identified Table B-1 of Fox et al. 2009 [ERMS 551679] as providing the basis for the parameter value, whereas the supporting documentation should have identified Table B-2 of that reference. SNL has agreed to correct this error. Other than this error, all forms were completely and correctly filled out.

## 7.0 REVIEW OF COMPUTING HARDWARE

Similar run structure and hardware were used for CRA-2009 and the PABC-2009 calculations. The calculations that were affected by the changes from PABC-2004 were updated, while the results from previous PAs were used for the calculations that were unaffected by the changes. For PABC-2009 calculations, the codes were executed on two computer systems, the WIPP PA Alpha Cluster and the WIPP PA Pentium 4 Cluster. These systems are described in the following tabulation and in Long 2010, Section 2 [ERMS 552947].

<b>Hardware Type</b>	<b>CPU</b>	<b>Operating System</b>
HP Alpha Server ES45 Model 2	Alpha EV68	Open VMS 8.2
HP Alpha Server ES47	Alpha EV7	Open VMS 8.2
Supermicro 4U dual processor rack mount server system	Intel Pentium 4 (Xeon)	Red Hat Enterprise Linux for Workstations, Version 4 (Kernel Release 2.6.9-11.ELsmp)
Supermicro 1U dial processor rack mount workstation systems	Intel Pentium 4 (Xeon)	Red Hat Enterprise Linux for Workstations, Version 4 (Kernel Release 2.6.9-11.ELsmp)

The WIPP PA Alpha Cluster consists of 8 Hewlett Packard (HP) AlphaServer nodes configured to share the same disk array using Storage Area Network (SAN) technology for efficient disk utilization and data storage and management. This allows for highly distributed processing while providing for integrated data access. The WIPP PA Pentium 4 Cluster consists of one Supermicro dual processor server node and 13 Supermicro dual processor computer nodes. Each computer node is configured to share the same disk on the server node.

The CRA-2009 PA was run on the same HP Alpha Servers as PABC-2009 (Long 2008 [ERMS 548350]). The Intel Pentium system was not used for CRA-2009, because it is only used for the MODFLOW runs and MODFLOW was not run for CRA-2009.

## 8.0 CONCLUSIONS

No significant database problems were identified in this review. Of the approximately 1,700 parameters in the PAPDB, 255 changes were made since 2004 that included 109 new parameters and 146 changes to the values of existing parameters. Most of the new parameters were introduced to either support new chemistry models or were replacements for parameters that were previously hand-coded into the input files for the performance assessment codes. The Agency has recommended transferring parameters to the PAPDB because of the enhanced traceability that the database provides. Changes to the values of existing parameters occurred primarily because of an update to the waste inventory that prompted not only inventory changes but also changes in solubility and density data. Other changes occurred due to updated hydrogeologic analyses and updated Delaware Basin drilling and plugging practices. All parameter distributions, values, and units were correctly entered into the PAPDB and were technically adequate and appropriate.

A check of primary and secondary supporting documents was made for all parameter changes and all documents were quickly retrieved from the WIPP Records Center. All documentation was found to be complete and accurate, with the single exception of a misidentified table that will be corrected by DOE. The outcome of this check supports a conclusion that the necessary documents are readily available to support the new and updated parameters. A database interface evaluation was performed for all new and changed parameters and the correct parameter values were retrieved from the PAPDB for each parameter. Changes to the performance assessment input file codes were reviewed for the presence of hand-coded parameter values with little traceability that would be better drawn from the PAPDB. Several parameters were moved into the PAPDB as a result of this review, and additional code comments were provided to enhance traceability for those hand-coded values used as numerical and run controls.

Updated procedures for developing, documenting, controlling, and changing parameters, and for entering those parameters into the PAPDB, were also reviewed. The Agency found all procedural changes to be consistent with earlier versions and found all revisions to be appropriate.

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