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TECHNICAL SUPPORT DOCUMENT FOR

SECTION 194.23: PARAMETER JUSTIFICATION REPORT

U. S. ENVIRONMENTAL PROTECTION AGENCY
Office of Radiation and Indoor Air
Center for the Waste Isolation Pilot Plant
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LIST OF ACRONYMS

BIR	Baseline Inventory Report
CCA	Compliance Certification Application
CCDF	Complementary Cumulative Distribution Function
CMS	Configuration Management System
DBR	Direct Brine Release
DOE	U.S. Department of Energy
DRZ	Disturbed Rock Zone
EEP	Expert Elicitation Panel
EPA	U.S. Environmental Protection Agency
JR	Parameter Justification Report
PA	Performance Assessment
PAVT	Performance Assessment Verification Test
PR	Parameter Report
QA	Quality Assurance
SA	Sensitivity Analysis
SNL	Sandia National Laboratories
TDEM	Time Domain Electromagnetic
WIPP	Waste Isolation Pilot Project

EXECUTIVE SUMMARY

This report describes the disposition of 58 Waste Isolation Pilot Project (WIPP) performance assessment (PA) input parameters that were found by the Agency to be inadequately supported. Each of these parameters was included in the database for the U.S. Department of Energy's (DOE) WIPP Compliance Certification Application (CCA) of October 1996. The finding of inadequate support was made by the Agency following a comprehensive review of nearly 1,600 parameters used in the WIPP PA. The inadequately supported parameters were identified to DOE in Enclosures 2, 3, and 4 of an Agency letter dated March 19, 1997, and many of those parameters were included in a sensitivity analysis performed by the Agency. The inadequately supported parameters were so identified because they were potentially important to the results of the PA and they lacked supporting data, they had different values or ranges than were supported in the DOE database, or they had questionable values or ranges.

Each of the inadequately supported parameters was further reviewed by the Agency and was either resolved and found to no longer be in question, or was included in the EPA-mandated Performance Assessment Verification Test (PAVT). A summary of the inadequately supported parameters and their disposition is presented in Tables ES-1 through ES-3. The mandated PAVT repeats the performance assessment calculations presented by DOE in the CCA but with modifications to the codes to correct errors identified by DOE and the Agency, and with revised values, ranges, and distributions determined by the Agency for those parameters that remained in question. Those parameters found to be no longer in question were typically either found to be not sensitive in the Agency's sensitivity analysis, the parameter was accepted after review of additional documentation provided by DOE or through the Agency's independent analysis, the parameter was eliminated because of a change in the model, or the parameter was found to not have been used in the CCA version of the PA model. In the last case, if the parameter or its use was considered by the Agency to be potentially important, alternate parameters were identified and changed in the PAVT to achieve the Agency's objective in questioning the original parameter.

After making the necessary adjustments to allow for model changes, a final list of 22 parameters that were to be changed in the PAVT was developed and is presented in Table ES-4. This table also summarizes the parameter values, ranges, and distributions used in the PAVT as well as the original values used in the CCA. The basis for selecting each parameter, value, range, and distribution is presented in Sections 3, 4, and 5 of this report.

Table ES-1. Parameters Lacking Supporting Data

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
1	3245	BLOWOUT-CEMENT	Waste cementation strength	Change required for PAVT in 4/25 letter but removed	Sensitive but removed due to change in model
2	3246	BLOWOUT-PARTDIA	Waste particle diameter	Required revision using expert elicitation process	Not appropriately justified
3	198	DRZ_1-PRMX_LOG	Intrinsic permeability in X-direction in disturbed rock zone	Change required for PAVT in 4/17 letter	Sensitive and not appropriately justified
4	2177	S_MB_139-DPHIMAX	Incremental increase in anhydrite porosity in Marker Bed 139	Removed in 4/25 letter	Documentation provided and accepted after review
5	2180	S_MB_139-PF_DELTA	Incremental pressure for full fracture development	Removed in 4/25 letter	Documentation provided and accepted after review
6	586	S_MB_139-PI_DELTA	Fracture initiation pressure increment	Removed in 4/25 letter	Documentation provided and accepted after review
7	2178	S_MB_139-KMAXLOG	Maximum permeability in altered anhydrite	Removed in 4/25 letter	Documentation provided and accepted after review
8	3134	BH_OPEN-PRMX_LOG	Intrinsic permeability in X-direction in open borehole	Removed in 4/25 letter	Not sensitive
9	2158	S_ANH_AB-DPHIMAX	Incremental increase in anhydrite porosity in beds A and B	Removed in 4/25 letter	Documentation provided and accepted after review
10	214	EXP_AREA-PRMX_LOG	Intrinsic permeability in X-direction in experimental area	Removed in 4/25 letter	Not sensitive
11	3473	BLOWOUT-THCK_CAS	Thickness of Castile brine pocket for direct brine release	Removed in 4/25 letter	Not sensitive
12	3456	BLOWOUT-RE_CAST	Radius of Castile brine pocket for direct brine release	Removed in 4/25 letter	Not sensitive
13	3194	CASTILER-GRIDFLO	Index for selecting brine pocket volume	Removed in 4/25 letter	Not used in CCA PA model - volume changed using other parameters

Table ES-2. Parameters with Different Values or Ranges

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
1	3493	GLOBAL-PBRINE	Probability of encountering pressurized brine	Change required for PAVT in 4/25 letter	Not appropriately justified
2	2254	BOREHOLE-TAUFAIL	Waste shear resistance	Change required for PAVT in 4/25 letter and 6/6 note to docket	Sensitive and not appropriately justified
3	3184	BH_SAND-PRMX_LOG	Long term intrinsic borehole permeability in X-direction	Change required for PAVT in 4/17 letter	Sensitive and not appropriately justified
4	2918	CASTILER-VOLUME	Castile brine pocket volume	Removed in 4/25 letter	Not used in CCA PA model - volume changed using compressibility and porosity adjustment
5	61	CASTILER-COMP_RCK	Castile brine pocket rock compressibility	Change required for PAVT in 4/17 letter	Not appropriately justified; used to change brine pocket volume

Table ES-3. Parameters with Questionable Values or Ranges

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
1	27	BOREHOLE-DOMEGA	Drill string angular velocity	Change required for PAVT in 4/25 letter	Sensitive and not appropriately justified
2	64	CASTILER-POROSITY	Castile brine pocket porosity	Removed in 4/25 letter	Not sensitive
3	66	CASTILER-PRESSURE	Castile brine pocket pore pressure	Removed in 4/25 letter	Not sensitive
4	259	PAN_SEAL-PRMX_LOG	Intrinsic permeability of panel seal in X-direction	Removed in 4/17 letter	Not sensitive
5	528	S_ANH_AB-POROSITY	Porosity of anhydrite beds A and B	Removed in 4/17 letter	Not sensitive
6	567	S_MB138-POROSITY	Porosity of anhydrite Marker Bed 138	Removed in 4/17 letter	Not sensitive
7	588	S_MB139-POROSITY	Porosity of anhydrite Marker Bed 139	Removed in 4/17 letter	Not sensitive
8	651	WAS_AREA-ABSROUGH	Waste area absolute roughness	Removed in 4/17 letter	Not sensitive and acceptable after review of documentation
9	653	WAS_AREA-COMP_RCK	Waste area rock compressibility	Removed in 4/17 letter	Not sensitive
10	1992	WAS_AREA-DIRNCCHW	Bulk density of iron containers in CH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review
11	1993	WAS_AREA-DIRNCRHW	Bulk density of iron containers in RH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review
12	2040	WAS_AREA-DIRNCHW	Average density of iron-based material in CH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review
13	2041	WAS_AREA-DCELLCHW	Average density of cellulosics in CH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review
14	2274	WAS_AREA-DCELLRHW	Average density of cellulosics in RH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review
15	2907	STEEL-CORRMCO2	Steel corrosion rate	Change required for PAVT in 4/17 letter	Not appropriately justified
16	3147	CONC_PLG-POROSITY	Borehole plug porosity	Removed in 4/17 letter	Not sensitive

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
17	3185	CONC_PLG-PRMX_LOG	Borehole plug permeability in X-direction	Change required for PAVT in 4/17 letter	Sensitive and not appropriately justified
18	3256	BLOWOUT-FGE	Gravity scaling factor	Change required for PAVT in 4/17 letter but removed	Removed due to change in model
19	3259	BLOWOUT-APORO	Waste permeability in CUTTINGS_S Model	Change required for PAVT in 4/25 letter but removed	Not used in CCA PA model -replaced with changes to parameters 663 WAS_AREA-PRMX_LOG and 2131 REPOSIT-PRMX_LOG
20	3429	PHUMOX3-PHUMCIM	Humic colloid proportionality constant	Removed in 4/25 letter	Not sensitive
21	3471	BLOWOUT-MAXFLOW	Maximum period of uncontrolled borehole flow	Removed in 4/25 letter	Sensitive, but documentation provided and accepted after review
22	3472	BLOWOUT-MINFLOW	Minimum period of uncontrolled borehole flow	Removed in 4/25 letter	Not sensitive
23	3433	PHUMOX3-PHUMSIM	Humic colloid proportionality constant	Removed in 4/25 letter	Not sensitive
24	3470	GLOWOUT-GAS_MIN	DBR cutoff gas flow rate	Removed in 4/25 letter	Not sensitive
25	3317	PU-PROPMIC	Microbial colloid proportionality constant for plutonium	Removed in 4/25 letter	Not sensitive
26	3405	SOLMOD6-SOLCIM	U(VI) solubility limit in Castile brine	Removed in 6/6 note to docket	Sensitive, but documentation provided and accepted after review
27	3409	SOLMOD6-SOLSIM	U(VI) solubility limit in Salado brine	Removed in 6/6 note to docket	Sensitive, but documentation provided and accepted after review
28a	3406	SOLMOD3-SOLCIM	Oxidation state +3 solubility limit in Castile brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
28b	3402	SOLMOD3-SOLSIM	Oxidation state +3 solubility limit in Salado brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
29	3403	SOLMOD4-SOLCIM	Oxidation state +4 solubility limit in Castile brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
30	3407	SOLMOD4-SOLSIM	Oxidation state +4 solubility limit in Salado brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
31	3404	SOLMOD5-SOLCIM	Oxidation state +5 solubility limit in Castile brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
32	3408	SOLMOD5-SOLSIM	Oxidation state +5 solubility limit in Salado brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
33	3311	AM-PROPMIC	Microbial colloid proportionality constant for americium	Removed in 4/25 letter	Not sensitive
34	3482	AM+3-MKD_AM	Matrix partition coefficient for americium +3	Change in distribution required for PAVT in 4/25 letter	Range accepted after review of documentation
35	3480	PU+3-MKD_PU	Matrix partition coefficient for plutonium +3	Change in distribution required for PAVT in 4/25 letter	Range accepted after review of documentation
36	3481	PU+4-MKD_PU	Matrix partition coefficient for plutonium +4	Change in distribution required for PAVT in 4/25 letter	Range accepted after review of documentation
37	3479	U+4-MKD_U	Matrix partition coefficient for uranium +4	Change in distribution required for PAVT in 4/25 letter	Range accepted after review of documentation
38	3478	TH+4 - MKD_TH	Matrix partition coefficient for thorium +4	Added to list, required for PAVT on 4/25 letter footnote. Changed distribution	Range accepted after review of documentation
39	3475	U+6-MKD_U	Matrix partition coefficient for uranium +6	Change in distribution required for PAVT in 4/25 letter	Range accepted after review of documentation
40	656	WAS_AREA-GRATMICH	Gas generation rate due to microbial action under humid conditions	Removed in 4/25 letter	No sensitivity
41	657	WAS_AREA-GRATMICI	Gas generation rate due to microbial action under inundated conditions	Removed in 4/25 letter	No sensitivity

Table ES-4. Parameters Changed by EPA in Performance Assessment Verification Test

ID No.	**Material ID - Parameter ID**	**Use**	**Distribution**	**Minimum**	**Maximum**	**Median**	**Units**
198	DRZ_1 - PRMX_LOG ◊	PAVT CCA	Uniform Constant	-19.4 -15.0	-12.5 -15.0	-15.95 -15.0	Log m^2 Log m^2
3184	BH_SAND - PRMX_LOG ◊	PAVT CCA	Uniform Uniform	-16.3 -14.0	-11.0 -11.0	-13.65 -12.5	Log m^2 Log m^2
3185	CONC_PLG - PRMX_LOG ◊	PAVT CCA	Uniform Constant	-19 -16.3	-17 -16.3	-17.3 -16.3	Log m^2 Log m^2
663	WAS_AREA - PRMX_LOG*◊	PAVT CCA	Constant Constant	-12.6198 -12.769	-12.6198 -12.769	-12.6198 -12.769	Log m^2 Log m^2
2131	REPOSIT - PRMX_LOG*◊	PAVT CCA	Constant Constant	-12.6198 -12.769	-12.6198 -12.769	-12.6198 -12.769	Log m^2 Log m^2
2907	STEEL - CORRMCO2	PAVT CCA	Uniform Uniform	0.0 0.0	3.17 E-14 1.59 E-14	1.58 E-14 7.94 E-14	m/s m/s
61	CASTILER - COMP_RCK	PAVT CCA	Triangular Triangular	2.0 E-11 5.0 E-12	1.0 E-10 1.0 E-08	4.0 E-11⌂ 1.0 E-10⌂	Pa^{-1} Pa^{-1}
8000	CASTILER - POR_BPKT ☆	PAVT CCA	Triangular - -	0.1848 - -	0.9240 - -	0.3696⌂ - -	Dimension-less
3493	GLOBAL - PBRINE	PAVT CCA	Uniform Constant	0.01 0.08	0.60 0.08	0.305 0.08	Dimension-less
27	BOREHOLE - DOMEGA	PAVT CCA	Cumulative Constant	4.20 7.8	23.0 7.8	7.8 7.8	Radians/sec Radians/sec
2254	BOREHOLE - TAUFAIL	PAVT CCA	Loguniform Uniform	0.05 0.05	77.0 10.0	2.0 5.025	Pa Pa
3482	AM+3 - MKD_AM	PAVT CCA	Loguniform Uniform	0.02 0.02	0.50 0.50	0.10 0.26	m^3/kg m^3/kg
3480	PU+3 - MKD_PU	PAVT CCA	Loguniform Uniform	0.02 0.02	0.50 0.50	0.10 0.26	m^3/kg m^3/kg
3481	PU+4 - MKD_PU	PAVT CCA	Loguniform Uniform	0.900 0.900	20.0 20.0	4.243 10.45	m^3/kg m^3/kg
3479	U+4 - MKD_U	PAVT CCA	Loguniform Uniform	0.900 0.900	20.0 20.0	4.243 10.45	m^3/kg m^3/kg
3475	U+6 - MKD_U	PAVT CCA	Loguniform Uniform	3.00 E-05 3.00 E-05	3.00 E-02 3.00 E-02	9.49 E-04 1.50 E-02	m^3/kg m^3/kg
3478	TH+4 - MKD_TH	PAVT CCA	Loguniform Uniform	0.900 0.900	20.0 20.0	4.243 10.45	m^3/kg m^3/kg

ID No.	Material ID - Parameter ID	Use	Distribution	Minimum	Maximum	Median	Units
3406	SOLMOD3 - SOLSIM	PAVT CCA	Constant Constant	1.2 E-07 5.82 E-08	1.2 E-07 5.82 E-08	1.2 E-07 5.82 E-08	moles/liter moles/liter
3402	SOLMOD3 - SOLCIM	PAVT CCA	Constant Constant	1.3 E-08 6.52 E-08	1.3 E-08 6.52 E-08	1.3 E-08 6.52 E-08	moles/liter moles/liter
3407	SOLMOD4 - SOLSIM	PAVT CCA	Constant Constant	1.3 E-08 4.4 E-06	1.3 E-08 4.4 E-06	1.3 E-08 4.4 E-06	moles/liter moles/liter
3403	SOLMOD4 - SOLCIM	PAVT CCA	Constant Constant	4.1 E-08 6.0 E-09	4.1 E-08 6.0 E-09	4.1 E-08 6.0 E-09	moles/liter moles/liter
3408	SOLMOD5 - SOLSIM	PAVT CCA	Constant Constant	2.4 E-07 2.3 E-06	2.4 E-07 2.3 E-06	2.4 E-07 2.3 E-06	moles/liter moles/liter
3404	SOLMOD5 - SOLCIM	PAVT CCA	Constant Constant	4.8 E-07 2.2 E-06	4.8 E-07 2.2 E-06	4.8 E-07 2.2 E-06	moles/liter moles/liter

* These parameters replaced BLOWOUT - APORO, which is not used in a current PA code
⌂ This is the mode of the triangular distribution
◊ Parameter similarly varied in Y- and Z-directions
☆ New parameter and number created by DOE for the PAVT to allow brine pocket volume to be varied

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1.0 INTRODUCTION

EPA conducted a comprehensive review of the supporting rationale for the parameters used in the performance assessment (PA) calculations presented by the U.S. Department of Energy (DOE) in the October 1996 Compliance Certification Application (CCA) for the Waste Isolation Pilot Plant (WIPP). Those parameters found to be inadequately supported were identified by the Agency to DOE in March 1997. This report identifies those parameters, presents the basis for their original selection, and describes the subsequent evaluations that were performed to identify the parameters of primary concern for regulatory compliance.

1.1 Background and Scope

This report is one of a series of three reports that provide detailed documentation of EPA's technical review of the CCA and the methodology used by the Agency to evaluate DOE compliance with the requirements of 40 CFR 194.23(c)(4). These three reports are briefly described in the following paragraphs.

The first report, *Technical Support Document for Section 194.23 - Parameter Report (PR)* [Docket A-93-02, Item V-B-12], describes EPA's detailed review of the DOE's supporting documentation and technical rationale for the parameters used in the PA model. The report describes the screening process used by the Agency to identify those parameters that were poorly documented, that had a weak technical basis, and that may be important in determining compliance. This screening occurred in several steps and culminated in identifying a series of parameters that warranted further review. Those parameters are listed Tables ES-1, ES-2, and ES-3 of this report.

The second report, *Technical Support Document for Section 194.23 - Sensitivity Analysis Report* (SA) [Docket A-93-02, Item V-B-13], describes the Agency's evaluation of key PA model outputs to changes in selected input parameters. The input parameters selected for this analysis were based primarily on the results of the Parameter Report (1998) and most of those parameters were identified to DOE in the aforementioned Agency letter of 19 March 1997 (Trovato 1997A). However, additional parameters or groups of parameters were added to the analysis based on the initial results of the Agency's sensitivity studies and on concerns for specific parameters and processes expressed during EPA's public hearings and in public written comments.

This third report, *Technical Support Document for Section 194.23 - Parameter Justification Report* [Docket A-93-02, Item V-B-14], is referred to as the Justification Report (JR). It describes the disposition of the inadequately supported parameters described in the Agency's letter of March 19, 1997 (Trovato 1997A). This disposition was based on the results of the Agency's sensitivity analysis, additional supporting information provided by the DOE, and further analysis by the Agency. Parameters were removed from the list by the Agency if, for example, PA performance measures were found to be insensitive to them, if the additional DOE supporting information was found to be adequate, or if upon further review the Agency determined that DOE’s existing supporting rationale was acceptable. The disposition of these parameters was described to DOE in the Agency’s letters of 17 April 1997 (Trovato 1997B) and 25 April 1997 (Trovato 1997C).

Parameters that were not removed from the list were used in developing a revised data base of parameters of major concern to the Agency for use in the EPA-mandated Performance Assessment Verification Test (PAVT). The rationale supporting development of this revised data base is presented in this report. The PAVT is designed to provide a comprehensive test of the effects of changes in significant, uncertain parameters and changes in other aspects of the CCA PA computer codes on the PA compliance calculations presented by DOE in the CCA.

1.2 Report Structure

This report is divided into six sections. Following this introduction, an overview of the parameter selection process is presented in Section 2. This overview describes the Agency’s review of parameter documentation, the screening process, and the sensitivity analysis process that were used to disposition the inadequately supported parameters. Sections 3, 4, and 5 present detailed discussions of the inadequately supported parameters listed in Enclosures 2, 3, and 4, respectively, of the Agency’s aforementioned letter of March 19, 1997 (Trovato 1997A). Finally, Section 6 presents a summary of the results of the Agency’s analysis of those parameters.

2.0 PARAMETER SELECTION PROCESS

2.1 Parameter Selection

The parameters identified to DOE as being inadequately supported were the result of a screening process described in the Parameter Report (1998). In overview, this process began with a detailed EPA review of the Sandia National Laboratories (SNL) parameter data base in Albuquerque, New Mexico. Individual Records Packages were obtained from SNL's Nuclear Waste Management Program Information Service Center and reviewed to identify the source and rationale for the principal parameters used in the CCA PA model. Deficiencies in documentation and lack of adequate rationale were identified and used along with information from the CCA and past SNL/DOE reports to begin an evaluation of parameter importance. This effort proceeded as a process of iterative sifting of the original CCA PA parameter database to identify those parameters deemed important to the performance of the WIPP.

The initial review involved nearly 1600 parameters. Of these, about 465 parameters were found to be worthy of a more detailed evaluation. These 465 parameters were given additional screening for importance and uncertainty, and about 150 were considered to have potential impact on performance. These 150 parameters were further reviewed and about 60 parameters were identified for inclusion in EPA's March 19, 1997 letter (Trovato 1997A). Those parameters were grouped by type of deficiency and are listed in Table 2.1-1.

2.2 Parameter Review

In the Agency's letter of March 19, 1997 (Trovato 1997A) the DOE was told that the issues described included EPA's outstanding concerns with the CCA and was requested to resolve those concerns. DOE responded by providing additional documentation and rationale which the Agency found helpful in evaluating many of the parameters. Additional information on many of the parameters was developed through technical reviews by the Agency and was also used to help in the evaluation process. Details of this additional documentation and rationale and the decisions they supported are presented in the parameter-by-parameter discussions in Sections 3 through 5 of this report.

Additionally, many of the inadequately supported parameters identified in the Agency's March 19, 1997 letter (Trovato 1997A) were selected by the Agency for detailed sensitivity analysis. These parameters, supplemented by others that were added later, totaled about 80 inputs that were evaluated in that analysis . PA model sensitivity to changes in both individual input parameters and groups of parameters was evaluated in 40 sensitivity analyses performed by the Agency. In most of these analyses, the parameters for which sensitivity was being analyzed were assigned low, high, and baseline values. The low and high values were selected by EPA to provide an indication of the changes in model output performance measures resulting from large and sometimes extreme changes, both up and down, in the input parameter values. The performance measures are model output parameters selected by the Agency that either directly represent or strongly influence radionuclide releases calculated in performance assessment and therefore serve as indicators of the importance of uncertainty in an input parameter to repository performance. An example performance measure is the calculated direct brine release, which directly represents a radionuclide release and is an output parameter of the BRAGFLO-DBR model. Another example performance measure is the calculated repository gas pressure, which is an output parameter of the BRAFGLO model and strongly influences spallings and brine releases during inadvertent borehole intrusions. In most cases, a percent change in a performance measure will result in a much smaller percent change in the total radionuclide release. The selection of performance measures for the SA is more fully discussed in Appendix PM of the SA Report (1998).

The baseline values for the sensitivity analysis were generally the values used by DOE in the CCA PA model or, in the case of sampled parameters, the median of the sampled range. The sensitivity analysis results were analyzed by calculating the average absolute percent change in the performance measure for the high and low parameter values. The results were found to range from zero to many thousand percent and were used to help select the inadequately supported parameters. The detailed results of this analysis are presented in the SA Report (1998).

Using additional information of the type described above, the Agency was able to conclude that many of the parameters were no longer in question. The supporting reasons for this finding included evidence from the SA that the PA model was not sensitive to changes in the value of the parameter, presentation by DOE of adequate supporting data for the parameter value, or development of adequate justification for the parameter value or range by DOE or through the Agency's own studies. Those parameters that were not included in this category were given alternative values that were considered by the Agency to be more appropriate. The Agency required DOE to use these alternative values in the PAVT, as stated in the Agency's letters of 17 April 1997 (Trovato 1997B) and 25 April 1997 (Trovato 1997C). For those parameters that were changed in the PAVT, the Agency's rationale for selecting the mandated alternative values is presented in Sections 3 through 5 of this report.

Table 2.1-1
Inadequately Supported Parameters Identified in EPA's March 19, 1997 Letter

No.	Parameter No.	Material ID - Parameter ID	Parameter Description
A. Parameters Lacking Supporting Data (Enclosure 2 Parameters)			
1	3245	BLOWOUT - CEMENT	Waste Cementation Strength
2	3246	BLOWOUT - PARTDIA	Waste Particle Diameter
3	198	DRZ_1 - PRMX_LOG	DRZ Permeability
4	2177	S_MB_139 - DPHIMAX	Incremental Increase in Anhydrite Porosity in MB 139
5	2180	S_MB_139 - PF_DELTA	Incremental Pressure for Full Fracture Development
6	586	S_MB_139 - PI_DELTA	Fracture Initiation Pressure Increment
7	2178	S_MB_139 - KMAXLOG	Maximum Permeability in Altered Anhydrite
8	3134	BH_OPEN - PRMX_LOG	Open Borehole Permeability
9	2158	S_ANH_AB - DPHIMAX	Incremental Increase in Anhydrite Porosity in Beds A and B
10	214	EXP_AREA - PRMX_LOG	Experimental Area Permeability
11	3473	BLOWOUT - THCK_CAS	Thickness of Castile Brine Pocket for Direct Brine Release
12	3456	BLOWOUT - RE_CAST	Radius of Castile Brine Pocket for Direct Brine Release
13	2918	CASTILER - GRIDFLO	Index for Selecting Brine Pocket Volume
B. Parameters with Different Values or Ranges (Enclosure 3 Parameters)			
1	3493	GLOBAL - PBRINE	Probability of Encountering Pressurized Brine
2	2254	BOREHOLE - TAUFAIL	Waste Shear Resistance
3	3184	BH_SAND - PRMX_LOG	Long-Term Borehole Permeability
4	2918	CASTILER - VOLUME	Castile Brine Pocket Volume
5	61	CASTILER - COMP_RCK	Castile Brine Pocket Rock Compressibility
C. Parameters with Questionable Values or Ranges (Enclosure 4 Parameters)			
1	27	BOREHOLE - DOMEGA	Drill String Angular Velocity
2	64	CASTILER - POROSITY	Castile Brine Pocket Porosity
3	66	CASTILER - PRESSURE	Castile Brine Pocket Pore Pressure
4	259	PAN_SEAL - PRMX_LOG	Panel Seal Permeability
5	528	S_ANH_AB - POROSITY	Effective Porosity of Anhydrite Beds A and B
6	567	S_MB138 - POROSITY	Effective Porosity of Anhydrite MB 138
7	588	S_MB139 - POROSITY	Effective Porosity of Anhydrite MB 139
8	651	WAS_AREA - ABSROUGH	Waste Area Absolute Roughness
9	653	WAS_AREA - COMP_RCK	Waste Area Rock Compressibility
10	1992	WAS_AREA - DIRNCCHW	Bulk Density of Iron Containers in CH Waste
11	1993	WAS_AREA - DIRNCRHW	Bulk Density of Iron Containers in RH Waste
12	2040	WAS_AREA - DIRNCHW	Average Density of Iron-Based Material in CH Waste
13	2041	WAS_AREA - DCELLCHW	Average Density of Cellulosics in CH Waste

Table 2.1-1
Inadequately Supported Parameters Identified in EPA's March 19, 1997 Letter
(Continued)

No.	Parameter No.	Material ID - Parameter ID	Parameter Description
14	2274	WAS_AREA - DCELLRHW	Average Density of Cellulosics in RH Waste
15	2907	STEEL - CORRMCO2	Steel Corrosion Rate
16	3147	CONC_PLG - POROSITY	Borehole Plug Porosity
17	3185	CONC_PLG - PRMX_LOG	Borehole Plug Permeability
18	3256	BLOWOUT - FGE	Gravity Scaling Factor
19	3259	BLOWOUT - APORO	Waste Permeability in CUTTINGS_S Model
20	3429	PHUMOX3 - PHUMCIM	Humic Colloid Proportionality Constant in Castile Brine
21	3471	BLOWOUT - MAXFLOW	Maximum Period of Uncontrolled Borehole Flow
22	3472	BLOWOUT - MINFLOW	Minimum Period of Uncontrolled Borehole Flow
23	3433	PHUMOX3 - PHUMSIM	Humic Colloid Proportionality Constant in Salado Brine
24	3470	BLOWOUT - GAS_MIN	DBR Cutoff Gas Flow Rate
25	3317	PU - PROPMIC	Microbial Colloid Proportionality Constant for Plutonium
26	3405	SOLMOD6 - SOLCIM	U(VI) Solubility Limit in Castile Brine
27	3409	SOLMOD6 - SOLSIM	U(VI) Solubility Limit in Salado Brine
28	3402	SOLMOD3 - SOLCIM	Oxidation State +3 Solubility Limit in Castile Brine
29	3403	SOLMOD4 - SOLCIM	Oxidation State +4 Solubility Limit in Castile Brine
30	3407	SOLMOD4 - SOLSIM	Oxidation State +4 Solubility Limit in Salado Brine
31	3404	SOLMOD5 - SOLCIM	Oxidation State +5 Solubility Limit in Castile Brine
32	34-8	SOLMOD5 - SOLSIM	Oxidation State +5 Solubility Limit in Salado Brine
33	3311	AM - PROPMIC	Microbial Colloid Proportionality Constant for Americium
34	3482	AM+3 - MKD_AM	Matrix Partition Coefficient for Americium +3
35	3480	PU+3 - MKD_PU	Matrix Partition Coefficient for Plutonium +3
36	3481	PU+4 - MKD_PU	Matrix Partition Coefficient for Plutonium +4
37	3479	U+4 - MKD_U	Matrix Partition Coefficient for Uranium +4
38	3475	U+6 - MKD_U	Matrix Partition Coefficient for Uranium +6
39	656	WAS_AREA - GRATMICH	Gas Generation Rate due to Microbial Action under Humid Conditions
40	657	WAS_AREA - GRATMICI	Gas Generation Rate due to Microbial Action under Inundated Conditions

3.0 PARAMETERS LACKING SUPPORTING DATA

Parameters for which the Agency was initially unable to find supporting data are addressed in this section. These parameters are listed in Enclosure 2 of the Agency's March 19, 1997 letter (Trovato 1997A). As stated in that letter, the Agency considers the traceability of the parameter and data record packages that support the input parameter values used in the PA to be important, and requires that the critical input parameters must either be supported by actual data collection and/or results of experimentation, or be based on expert judgement following the Agency's procedures. Each of the following subsection headings identifies the parameter's reference number, Material ID, and Parameter ID, followed by a brief description of the parameter. Parameter values are often presented in the format used for model input and very large or very small numbers may be expressed as logarithms. For example, the permeability 1.7 x 10^{-13} m^2 may be expressed as $\log_{10}$ 1.7 E-13 m^2 or -12.769 log m^2.

3.1 3245 BLOWOUT - CEMENT: Waste Cementation Strength

The waste cementation strength was used in the CUTTINGS_S code for predicting spallings releases. It is a measure of the strength imparted to the waste by cementitious materials that are expected by DOE to form in waste pores due to the precipitation of salts in the repository brine. The cement is expected to be primarily derived from precipitation and redeposition of halite, MgO reaction products, and corrosion reaction products around waste particles during the life of the repository. This parameter is not supported by data collection or experimentation, nor was it developed by expert judgement following the Agency's procedures (see WPO # 38241). This parameter was reviewed by DOE's Engineered Systems Peer Review Panel, which stated that its value was highly uncertain and could range from near zero to 700 psi and recommended treating it as a sampled variable in the PA (Ross-Brown et al. 1996 p. 16). Additionally, at the time the Agency's March and April letters to DOE were prepared (Trovato 1997A; 1997B; 1997C), the spallings release model had not been approved by the DOE's Conceptual Models Peer Review Panel (Wilson et al. 1997A p. 2ff). Because of its uncertainty and potential significance in computing spallings releases, this parameter was identified for further evaluation.

Waste cementation strength was included in the Agency's sensitivity analysis and given a high value that was 700 times the value used in the CCA PA. The average absolute change for this parameter was found to be 149%. Although this sensitivity is low compared with results for other parameters, it exceeded the Agency's threshold value of 25%. Partially because of the demonstrated sensitivity of spallings releases to this parameter, but primarily because of the importance of spallings releases relative to total repository releases, a lack of confidence in the spallings release calculations, a lack of documented support for the adopted parameter value, and the high degree of uncertainty surrounding the correct parameter value, waste cementation strength was retained as a mandated, sampled variable for the PAVT (Trovato 1997C Enclosure 2).

For the PAVT, waste cementation strength was mandated in the Agency's letter of April 25, 1997 to be treated as a sampled variable with a log-uniform distribution, a minimum value equal to the minimum value to be set for the waste shear resistance (parameter BOREHOLE - TAUFAIL), and a maximum value of 4.8 E+06 Pa (see Trovato 1997C Enclosure 2). A log-uniform distribution was selected for this parameter because, based on present knowledge, the Agency believes that all values across the range of several orders of magnitude are equally likely. The minimum value was set equal to the minimum value of the waste shear resistance used in CUTTINGS_S to calculate cavings releases, based on the rationale that both parameters are a measure of the resistance of waste to the shear forces imposed by a fluid moving over the waste surface and there was no evident reason why the minimum value of the two parameters should be different. The maximum value was set equal to the upper end of the strength range recommended by the aforementioned Engineered Systems Peer Review Panel and is equal to 700 psi, which is the approximate strength of sorel cement.

DOE's Conceptual Models Peer Review Panel issued its final report at about the time that the foregoing data requirements were transmitted by the Agency to DOE. In that report the Panel continued to find the spallings conceptual model to be inadequate, but determined that the spallings volumes used by DOE in the CCA (0.5 to 4.0 m^3 per spall event) were reasonable for purposes of performance assessment (Wilson et al. 1997B p. 12). In view of this, DOE proposed and the Agency accepted that for the PAVT the spallings model would be changed to directly sample releases across the Panel's approved range from a uniform distribution rather than calculate those releases with the computational model. Although this change eliminated the need to vary the waste cementation strength parameter in the PAVT, its acceptance by the Agency was conditioned on the demonstration that the waste particle diameter distribution used by DOE in the CCA is more conservative (that is, addresses smaller particles) than the distribution resulting from expert judgement (see Section 3.2 below).

3.2 3246 BLOWOUT - PARTDIA: Waste Particle Diameter

The waste particle diameter was used in the CUTTINGS_S model to calculate spallings releases and to determine the waste shear resistance for calculating cavings releases. The waste particle diameter was identified in the Agency's letter of March 19, 1997 as lacking supporting evidence (Trovato 1997A Enclosure 2), and was further discussed in the Agency's letter of April 25, 1997 as not being supported by data and therefore requiring derivation through "expert judgement" (Trovato 1997C p. 1). The Agency considers expert elicitation (or expert judgement) to be an appropriate method for obtaining values of parameters that are not readily measurable or are highly uncertain and are therefore not supported by an extensive database. In summary, the method consists of convening a panel of acknowledged experts in a variety of fields associated with aspects of the parameters of concern who each contribute toward a final judgement regarding the parameter values. The advantage of the method is that for such parameters, the values can be selected to reflect probable sources of error in measurement, modeling, and the use of analogs from other sites, and the ranges can be selected to reflect the uncertainties in the parameter values. The alternative of basing parameter values only on available data without the benefit of judgement requires an extensive data base to assure that the values and associated uncertainties are adequately represented. In response to the Agency's mandate, the DOE convened an Expert Elicitation Panel (EEP) to derive values for waste particle diameters appropriate for use in WIPP PA. The results of that elicitation process are documented in the EEP's final report (DOE Carlsbad Area Office 1997).

DOE's analysis of the EEP's findings are summarized in an August 5, 1997 memorandum (WPO # 46936), wherein a bounding calculation is described that correlates the distributions derived by the EEP to the mean particle diameters used in the cavings and spallings models. Converting the EEP's particle size distributions to a volume fraction basis and considering complete waste degradation as a worst case, DOE calculated a lower bound mean diameter of 0.1 cm and an upper bound mean diameter ranging from 10 cm (the initial mean particle size, assuming no cementation) to the size of the waste panel (assuming that reacted MgO precipitates as a cement). The particle diameters were sampled from a log-uniform distribution in the CCA PA and ranged from 0.004 cm to 20 cm with a median value of 0.28 cm. The Agency accepted DOE's analysis as adequately demonstrating that the waste particle diameter distribution used in the CCA addresses smaller particles and is therefore more conservative than the distribution resulting from expert judgement. Calculations based on smaller particle sizes are more conservative because they result in greater radionuclide releases. Based on this determination, the Agency accepted the spallings model change described in Section 3.1, which eliminated the use of particle size information in determining spallings releases.

As previously mentioned, the waste particle diameter is used in the cuttings release calculations to determine waste shear resistance (parameter BOREHOLE - TAUFAIL). That parameter was identified as being inadequately supported in Enclosure 3 of the Agency's letter of March 19, 1997 (Trovato 1997A). Use of the EEP's waste particle size distributions in developing alternate values for that parameter is discussed in Section 4.2 of this report.

3.3 198 DRZ_1 - PRMX_LOG: DRZ Permeability

The DRZ permeability is the permeability in the X-direction of the disturbed rock zone (DRZ) surrounding the repository. This parameter, entered into the PA database as a logarithm, was assumed to be a constant equal to -15 log m^2 in the CCA PA. In Chapter 6, Section 6.4.5.3 DOE states that using a constant DRZ permeability is conservative. This parameter is potentially significant in computing spallings and direct brine releases because of its influence on repository gas pressure buildup. It was identified in the Agency's March 19, 1997 letter for further evaluation (Trovato 1997A Enclosure 2).

The DRZ permeability was included in the Agency's sensitivity analysis where it was given a high value of 12.5 log m^2 and a low value of -21 log m^2 (see SA Report 1998 Appendix PD Section PD-3.12). These values were determined by the Agency based on the maximum and minimum of 14 field permeability measurements within the DRZ of the WIPP excavations (see WPO # 32038 Rev 1 p. 2). The average absolute change in the performance measures for this parameter was found to be 325%, which the Agency considered potentially significant (see SA Report 1998 Table 3.1-1). Because of the demonstrated sensitivity of the PA model results to this parameter and because of the potential importance of this parameter in calculating gas pressure buildup in the repository, alternate values were identified for this parameter and its Y-and Z-direction counterparts in the Agency's April 17, 1997 letter for use in the PAVT (Trovato 1997B Enclosure 2).

The DRZ log permeabilities specified by the Agency for use in the PAVT ranged from a low of -19.4 log m^2 to a high of -12.5 log m^2, to be sampled from a uniform distribution with a median of -15.95 log m^2 (see Trovato 1997B Enclosure 2 and Kruger 1997). The low end of the range is based on the lowest value measured by DOE in gas permeability tests in anhydrite cores from Marker Bed 139 (see WPO # 30603 p. 2 and WPO # 32038). The test samples were disturbed by the drilling and sample preparation processes (see WPO # 38367 p. 11) and the Agency believes that the lowest of those measured permeabilities provides an appropriate lower bound for sampling DRZ permeability in the PAVT. The high end of the range is the same as the high value of the sensitivity analysis and is based on the reasoning described above. A uniform distribution was selected for the log-permeabilities because, based on present knowledge, the Agency believes that all values across the range of several orders of magnitude are equally likely. The median value is determined from the type and range of the distribution. This mandated approach is considered by the Agency to adequately reflect both the uncertainty and the reasonable range of values for this parameter. The variation of this parameter in the PAVT is expected to result in a greater range of computed spallings and direct brine releases because of its influence on repository gas pressure buildup. The lower median permeability in the PAVT is expected to conservatively result in higher direct brine releases because the restricted gas migration may result in higher repository gas pressures.

3.4 2177 S_MB_139 - DPHIMAX: Maximum Incremental Increase in Anhydrite Porosity in Marker Bed 139

Porosity was allowed to increase in the anhydrite interbeds near the repository in response to increases in gas/brine pressure in the repository. Parameter S_MB_139 - DPHIMAX was used to establish the maximum incremental porosity increase that would be allowed in anhydrite Marker Bed 139. It was treated as a constant in the CCA PA equal to 0.039. In its initial review, the Agency did not find this parameter to be supported by data collection or experimentation documented in the CCA or SNL WIPP records center, nor was it developed by expert judgement following the Agency's procedures. This parameter is potentially significant in computing brine releases through MB 139 to the accessible environment and was identified in the Agency's March 19, 1997 letter for further evaluation (Trovato 1997A Enclosure 2).

Anhydrite porosity was selected by the Agency for sensitivity analysis to determine whether PA model results were sensitive to changes in this and other parameters used in determining the value of that porosity. In that sensitivity analysis, DOE's initial, undisturbed anhydrite porosity of 0.011 was given a low value of 0.006 and a high value of 0.017 in all interbeds. These values were determined by the Agency based on the minimum and maximum porosities measured by DOE in 16 samples collected from the WIPP Site (see WPO # 34860 p. 2). The results of the sensitivity analysis showed no sensitivity of the model performance measures to changes in this parameter (see SA Report 1997 Table 3.1-1). Because of the lack of sensitivity to changes in anhydrite porosity for the range of values defined by the Agency in this analysis, additional sensitivity studies addressing the higher maximum porosity of 0.05 (equal to 0.011 + 0.039) defined by the parameter S_MB_139 - DPHIMAX were not considered necessary.

In addition to the results of the sensitivity analysis for anhydrite porosity, in a letter dated April 15, 1997 (Docket: A-93-02, II-I-24, Comment No. 9, Larson et al.1997) the Agency received additional information from DOE describing the use of experimental data in developing the anhydrite fracture generation parameters including those discussed in Sections 3.4 through 3.7 and 3.9 of this report. This letter and its attachments provided a list of the relevant contemporaneous documentation and a summary that provided a historical perspective of the development of the conceptual model and its implementing parameters and data base. Upon review, this information was found to provide an acceptable explanation of the experimental basis for the anhydrite fracture generation parameters addressed in this report.

As part of its review of this and the related anhydrite interbed parameters discussed in Sections 3.5 through 3.7 and 3.9 below, the Agency evaluated the appropriateness of the pressure-dependent porosity model used in the CCA compared with an alternative pressure-dependent aperture model (see Freeze et al. 1995 p. 6-25). The porosity model treats the anhydrite interbed as an equivalent porous medium and simulates the effect of fracturing by increasing both porosity (to increase storage) and permeability (to increase flow). DOE structured the porosity model with exponential terms to simulate the rapid rise in permeability accompanying fracturing. The aperture model addresses both increasing storage and flow by directly simulating propagation of an open fracture. The two models are capable of producing similar solutions for permeability changes and both have been used to match field data on permeability versus pore pressure (see Beauheim et al.1994 Figure 20). However, the models do not provide similar permeability/porosity correlations and for a given porosity change the aperture model predicts a higher permeability than the porosity model. Based on the pervasive presence of natural fractures in the anhydrite interbeds and on the results of hydrofracturing tests conducted at the WIPP Site by DOE, the Agency believes that the porosity model better represents conditions in the WIPP interbeds than the aperture model (see Beauheim et al. 1993). In view of DOE’s use of field and experimental data to select the model parameters, the Agency considers the application of the porosity model in the CCA to be reasonable.

In view of the acceptability of the additional information provided by DOE and the lack of model sensitivity to changes in anhydrite porosity, this parameter was identified in the Agency’s April 25, 1997 letter as being no longer in question (Trovato 1997C Enclosure 1).

3.5 2180 S_MB_139 - PF_DELTA: Incremental Pressure for Full Fracture Development in Marker Bed 139

Permeability and porosity were both allowed to increase in the anhydrite interbeds near the repository in response to increases in gas/brine pressure in the repository. Although fracture development was not specifically modeled, the process was conceptually considered to be analogous to hydrofracturing. This parameter was used to establish the incremental increase in repository pressure in Marker Bed 139 above the initial pressure in the anhydrite that would correlate to the maximum allowable permeability and porosity values. This parameter was treated as a constant in the CCA PA equal to 3.8 E+06 Pa. In its initial review, the Agency did not find this parameter to be supported by data collection or experimentation, nor was it developed by expert judgement following the Agency’s procedures. This parameter is potentially significant in computing brine releases through MB 139 to the accessible environment and was identified in the Agency’s March 19, 1997 letter for further evaluation (Trovato 1997A Enclosure 2).

To assess the sensitivity of the PA model to changes in this parameter, the Agency performed three sensitivity analyses that independently changed anhydrite porosity, permeability, and pressure. The sensitivity analysis for anhydrite porosity is discussed in Section 3.4 above and indicated no sensitivity of the model performance measures to changes in porosity.

The sensitivity analysis for anhydrite permeability was performed using a low value of -12 log m^2 and a high value of -17.1 log m^2 (see SA Report 1998 Appendix PD Section PD-1.1). Anhydrite permeability was treated by DOE as a sampled variable in the CCA with a Student T distribution, a median of -18.89 log m^2, and a range equal to the high and low values used by the Agency in its sensitivity analysis. These values were based on direct field measurements (see CCA, Volume XI, Appendix PAR p. PAR-81 [Docket: A-93-02, II-G-1]). This analysis showed a 2347% average change in the performance measures, which the Agency considers to be significant (see SA Report 1998 Table 3.1-1).

The sensitivity analysis for anhydrite initial pressure was performed using a low value of 1.1 E+07 Pa and a high value of 1.38 E+07 Pa (see SA Report 1998 Appendix PD Section PD-1.3). Anhydrite pressure was treated by DOE as a sampled variable in the CCA with a uniform distribution and a range equal to the high and low values used by the Agency in its sensitivity analysis. These values were based on direct field measurements (see CCA, Volume XI, Appendix PAR p. PAR-99 [Docket: A-93-02, II-G-1]). This analysis showed a 10% average change in the performance measures, which the Agency does not consider to be significant (see SA Report 1998 Table 3.1-1). For most parameters evaluated in the sensitivity analysis including the anhydrite initial pressure, the percent change in the overall radionuclide release will be considerably less than the percent change in the performance measures. The performance measures used in the sensitivity analysis are fully described in the SA Report.

Of the three parameters related to parameter S_MB_139 - PF_DELTA that were studied in sensitivity analysis, the model performance measures were only sensitive to changes in anhydrite permeability. Despite this demonstrated sensitivity, anhydrite permeability was not identified by the Agency as requiring changed values in the PAVT because the anhydrite permeability values upon which DOE based its analysis are extensive, appropriate, well documented, and were collected under an NQA-1 QA program. They are based on 5 in situ hydraulic tests and 31 laboratory tests from anhydrite interbeds in the Salado, and screened for both scale effects and repository-induced disturbance (see CCA, II-G-1, Volume XI, Appendix PAR p. PAR-81 [Docket: A-93-02, II-G-1]). The Agency considers DOE's treatment of anhydrite permeability in the CCA to adequately capture the expected value and uncertainty in this parameter.

In addition to the results of the foregoing sensitivity analyses, in a letter dated April 15, 1997 the Agency received additional information from DOE (Larson et al.1997) describing the use of experimental data in developing the anhydrite fracture generation parameters including those discussed in Sections 3.4 through 3.7 and 3.9 of this report. This letter is further discussed in Section 3.4 and was found to provide an acceptable explanation of the experimental basis for the anhydrite fracture generation parameters addressed in this report.

In view of the acceptability of the additional information provided by DOE, the results of the sensitivity analyses, and the acceptability of DOE's anhydrite permeability database, the parameter S_MB_139 - PF_DELTA was identified in the Agency's April 25, 1997 letter as being no longer in question (Trovato 1997C Enclosure 1).

3.6 586 S_MB_139 - PI_DELTA: Fracture Initiation Pressure Increment in Marker Bed 139

As described in Section 3.5, permeability and porosity were both allowed to increase in the anhydrite interbeds near the repository in response to increases in gas/brine pressure in the repository. This parameter was used to establish the minimum incremental increase in repository pressure above the initial pressure in the anhydrite that would initiate increases in the permeability and porosity of Marker Bed 139. This parameter was treated as a constant in the CCA PA equal to 0.2 E+06 Pa. In its initial review, the Agency did not find this parameter to be supported by data collection or experimentation, nor was it developed by expert judgement following the Agency's procedures. This parameter is potentially significant in computing brine releases through MB 139 to the accessible environment and was identified in the Agency's March 19, 1997 letter for further evaluation (Trovato 1997A Enclosure 2).

The Agency evaluated the sensitivity of PA model performance measures to changes in anhydrite interbed pressure by assigning low and high values to the initial value of that pressure. This sensitivity analysis is described in Section 3.5 above and indicated only a minor sensitivity to changes in this parameter. In addition to the results of the foregoing sensitivity analysis, in a letter dated April 15, 1997 the Agency received additional information from DOE (Larson et al.1997) describing the use of experimental data in developing the anhydrite fracture generation parameters including those discussed in Sections 3.4 through 3.7 and 3.9 of this report. This letter is further discussed in Section 3.4 and was found to provide an acceptable explanation of the experimental basis for the anhydrite fracture generation parameters addressed in this report.

In view of the acceptability of the additional information provided by DOE and the results of the sensitivity analysis, the parameter S_MB_139 - PI_DELTA was identified in the Agency's April 25, 1997 letter as being no longer in question (Trovato 1997C Enclosure 1).

3.7 2178 S_MB_139 - KMAXLOG: Maximum Permeability in Altered Anhydrite in Marker Bed 139

As described in Section 3.5, permeability was allowed to increase in the anhydrite interbeds near the repository in response to increases in gas and brine pressure in the repository. This parameter was used to establish the maximum log permeability in Marker Bed 139 that the model would allow to occur in response to increased repository pressures. This parameter was treated as a constant in the CCA PA equal to -9 log m^2. In its initial review, the Agency did not find this parameter to be supported by data collection or experimentation, nor was it developed by expert judgement following the Agency's procedures. This parameter is potentially significant in computing brine releases through MB 139 to the accessible environment and was identified in the Agency's March 19, 1997 letter for further evaluation (Trovato 1997A Enclosure 2).

In a letter dated April 15, 1997 the Agency received additional information from DOE (Larson et al.1997) describing the use of experimental data in developing the anhydrite fracture generation parameters including those discussed in Sections 3.4 through 3.7 and 3.9 of this report. This letter is further discussed in Section 3.4 and was found to provide an acceptable explanation of the experimental basis for the anhydrite fracture generation parameters addressed in this report.

In view of the acceptability of the additional information provided by DOE this parameter was identified in the Agency's April 25, 1997 letter as being no longer in question (Trovato 1997C Enclosure 1).

3.8 3134 BH_OPEN - PRMX_LOG: Open Borehole Permeability

The open borehole permeability is the permeability assigned to the unplugged parts of an intrusion borehole during the 200-year period before the borehole is assumed to be filled with casing corrosion products and material sloughed from the borehole walls. This parameter was treated as a constant in the CCA PA equal to -9 log m^2. In its initial review, the Agency did not find this parameter to be supported by data collection or experimentation, nor was it developed by expert judgement following the Agency's procedures. This parameter is potentially significant in computing long term brine releases through an intrusion borehole to the ground surface and was identified in the Agency's March 19, 1997 letter for further evaluation (Trovato 1997A Enclosure 2).

The open borehole permeability was one of the parameters selected by the Agency for sensitivity analysis. In that analysis, DOE's log permeability value was increased to -6 log m^2 . The Agency's objective was to determine the effect of a higher permeability value, and the low value was therefore set equal to the baseline CCA value. The SA results showed no sensitivity to this three order of magnitude increase in open borehole permeability (see SA Report 1998 Table 3.1-1). Because of a lack of sensitivity, this parameter was identified in the Agency's April 25, 1997 letter as being no longer in question (Trovato 1997C Enclosure 1).

3.9 2158 S_ANH_AB - DPHIMAX: Incremental Increase in Anhydrite Porosity in Beds A and B

This parameter applies to anhydrite beds A and B and is the same as defined for Marker Bed 139 in Section 3.4. It was treated as a constant in the CCA PA equal to 0.239. This value was selected by DOE to maintain equal transmissivities in all anhydrite interbeds in the porous medium model during the conceptual hydrofracturing process. Through the porosity-permeability correlation in the model it accounts for differences in thickness between anhydrite beds A and B and Marker Bed 139. The value of this parameter is therefore tied to the value of the parallel parameter for Marker Bed 139. In its initial review, the Agency did not find this parameter to be supported by data collection or experimentation, nor was it developed by expert judgement following the Agency's procedures. This parameter is potentially significant in computing brine releases through anhydrite beds A and B to the accessible environment and was identified in the Agency's March 19, 1997 letter for further evaluation (Trovato 1997A Enclosure 2). Because of its relationship to the aforementioned parallel parameter for Marker Bed 139, the Agency found parameter S_ANH_AB - DPHIMAX to be no longer in question for the reasons given for parameter S_MB_139 - DPHIMAX in Section 3.4. This finding is documented in the Agency's April 25, 1997 letter (Trovato 1997C Enclosure 1).

3.10 214 EXP_AREA - PRMX_LOG: Experimental Area Permeability

The WIPP repository excavations may be divided into the waste disposal area, the operations area, and the experimental area. The experimental area permeability is the permeability assigned in the PA model to the experimental area of the repository. This area and the operations area will not be filled with waste and will be allowed to close naturally through halite creep upon repository closure. This parameter was treated as a constant in the CCA PA equal to -11 log m^2 and was the same as the permeability assigned to the operations area. In its initial review, the Agency did not find this parameter to be supported by data collection or experimentation, nor was it developed by expert judgement following the Agency's procedures.

The experimental and operations area permeabilities were varied together in a sensitivity analysis conducted by the Agency. In that analysis, DOE's log permeability value was decreased to -17 log m^2. The Agency's objective was to determine the effect of a lower permeability value, and the high value was therefore set equal to the baseline CCA value. The SA results showed no sensitivity to this six order of magnitude decrease (see SA Report 1998 Table 3.1-1). Because of a lack of sensitivity, this parameter was identified in the Agency's April 25, 1997 letter as being no longer in question (Trovato 1997C Enclosure 1).

3.11 3473 BLOWOUT - THCK_CAS: Thickness of Castile Brine Pocket for Direct Brine Release

The parameters BLOWOUT - THCK_CAS and BLOWOUT - RE_CAST (see Section 3.12) were used in the PA model to define the thickness and radius, respectively, of a Castile brine pocket for the Direct Brine Release (DBR) model. The Castile brine pocket volume was treated as a constant in the CCA PA with an equivalent thickness equal to 12.34 m and an equivalent radius equal to 114 m. The thickness is based on the estimated thickness of the Castile anhydrite beds underlying the site that are believed by DOE to potentially contain brine pockets, and the equivalent radius of 114 m approximates the area of a waste panel. In its initial review, the Agency did not find this parameter to be supported by data collection or experimentation, nor was it developed by expert judgement following the Agency's procedures. During this review the Agency found that the equivalent radius used in the CCA was in error and that 230 m provided a more appropriate estimate of the actual area of a waste panel as documented by DOE in the documentation on direct brine release calculations. This parameter is potentially significant in computing direct brine releases through intrusion boreholes to the ground surface and was identified in the Agency's March 19, 1997 letter for further evaluation (Trovato 1997A Enclosure 2).

The parameters BLOWOUT - THCK_CAS and BLOWOUT - RE_CAST were varied together in a sensitivity analysis conducted by the Agency. In that analysis, the low brine pocket volume was assigned a thickness of 24 m and an equivalent radius of 30 m. These correspond to a gross volume of about 68,000 m^3. A thickness of 24 m is the maximum thickness of the Castile anhydrite beds believed by DOE to potentially contain brine pockets, and an equivalent radius of 30 m approximates the area of a single waste disposal room and surrounding salt pillars. The high brine pocket volume was assigned a thickness of 7 m and an equivalent radius of 230 m, corresponding to a gross volume of about 1,163,000 m^3. A thickness of 7 m is the minimum thickness of the Castile anhydrite beds believed by DOE to potentially contain brine pockets, and based on the corrected equivalent radius of 230 m approximates the area of two waste panels. For comparison, DOE's CCA PA dimensions correspond to a gross volume of about 500,000 m^3. By coupling the largest thickness with the smallest radius for the low volume, and the smallest thickness with the largest radius for the high volume, a range of volumes was achieved that the Agency considers appropriate for evaluating the sensitivity of DBR model results to changes in brine pocket volume. The SA results showed no sensitivity to these volume changes (see SA Report 1998 Table 3.1-1). Because of a lack of sensitivity, both BLOWOUT - THCK_CAS and BLOWOUT - RE_CAST were identified in the Agency's April 25, 1997 letter as being no longer in question (Trovato 1997C Enclosure 1).

3.12 3456 BLOWOUT - RE_CAST: Radius of Castile Brine Pocket for Direct Brine Release

This parameter is discussed along with BLOWOUT - THCK_CAS in Section 3.11. Because of a lack of sensitivity, both BLOWOUT - THCK_CAS and BLOWOUT - RE_CAST were identified in the Agency's April 25, 1997 letter as being no longer in question (Trovato 1997C Enclosure 1).

3.13 2918 CASTILER - GRIDFLO: Index for Selecting Brine Pocket Volume

The parameter CASTILER - GRIDFLO is an index for selecting the brine pocket volume in the BRAGFLO code. This parameter was treated as a sampled variable in the CCA PA ranging from 1 to 32. A CASTILER - GRIDFLO value of 1 selects the smallest volume pocket (pore volume of 32,000 m^3), and a value of 32 selects the largest volume pocket (pore volume of 160,000 m^3). An explanation of DOE's rationale for this parameter is presented in Section PD-1.9 of the SA Report (1998). In its initial review, the Agency did not find this parameter to be adequately supported. This parameter is potentially significant in computing brine releases associated with Castile brine pockets and was identified in the Agency's March 19, 1997 letter for further evaluation (Trovato 1997A Enclosure 2).

One of the analyses initially planned by the Agency was to test model sensitivity to the extreme values of the CCA brine pocket volume range. This analysis is described in Section PD-1.9 of the SA Report (1998). Simultaneously, the Agency tested model sensitivity to much larger volumes (3,400,000 m^3 to 17,000,000 m^3) as described in Section PD-1.10 of the SA Report (1998). When the sensitivity to the larger volumes was found to be only 1% (see SA Report 1998 Table 3.1-1), further evaluation of the smaller CCA range of brine pocket volumes was discontinued due to a low sensitivity and the parameter CASTILER - GRIDFLO was identified in the Agency's April 25, 1997 letter as being no longer in question (Trovato 1997C Enclosure 1). Additional discussion of the Castile brine pocket volume is presented in Section 4.5 of this report.

4.0 PARAMETERS WITH DIFFERENT VALUES OR RANGES

Parameters for which the Agency reviewed the supporting information and found that the information in the record supported a value or range of values different from those selected by DOE are addressed in this section. These parameters are listed in Enclosure 3 of the Agency's March 19, 1997 letter (Trovato 1997A). Each of the following subsection headings identifies the parameter's number, Material ID, and Parameter ID, followed by a brief description of the parameter.

4.1 3493 GLOBAL - PBRINE: Probability of Encountering Pressurized Brine

This parameter was used in the CCDFGF code for determining the frequency with which a pressurized Castile brine pocket would be encountered by an intrusion borehole. This parameter was treated as a constant in the CCA PA equal to 0.08, based on the results of a geostatistical analysis of pressurized brine pocket encounters in the vicinity of the WIPP Site (see WPO # 40199 p. 36). Additional quantitative information from the results of time domain electromagnetic (TDEM) geophysical surveys at the Site did not appear to have been used and supported a higher value for this parameter than was used by DOE in the CCA PA (The Earth Technology Corporation 1988 and A-93-02, Reference #563, Volume 3, Chapter 6, Table 6.0-3). Although the authors of the geophysical report did not provide an estimated value for this parameter, in a subsequent analysis of the TDEM data by SNL, the value of this parameter was estimated to range from 0.10 to 0.55 with an expected value of 0.25, depending on the depth of the pocket in the Castile (see WPO # 39121 p. 2). The DOE believes that the value of this parameter is lower than that inferred from the geophysical results because of the reduced probability of hitting subvertical fractures containing the brine with vertical boreholes. However, this argument was not used in a quantitative manner to support the lower parameter value. This parameter has a potentially significant influence on the amount of brine that could enter the repository and affect direct brine releases and spallings releases during drilling. It was therefore listed in Enclosure 3 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the probability of encountering pressurized brine in the Castile was studied in the Agency's SA using a low probability value of 0.01 and a high value of 0.60 (see SA Report 1998 Appendix PD Section PD-5.1). The Agency assigned a relatively broad range of values to this parameter to reflect its high degree of uncertainty.

The low value was selected by the Agency to represent a reasonable minimum that bounded the 1992 PA and the geostatistical study. The Agency believes that the DOE's geostatistical analysis, the aforementioned subvertical fracture hypothesis, and the low end of the range identified in WPO # 39121 have some merit, and while there is reasonable evidence that one or more brine pockets may be present beneath the site based on the TDEM data, it is not certain (i.e. a probability of 1) that a borehole penetrating such a geophysical anomaly would actually encounter pressurized brine with sufficient productivity to affect waste isolation. The Agency therefore believes that the true probability of encountering pressurized brine beneath the WIPP waste area could be low, and considers 0.01 to be a reasonable lower bound.

The high value was developed in consideration of the TDEM data and represents a reasonable maximum in view of the aforementioned alternative interpretations that have been based on these data (see WPO # 40199 p. 36 and WPO # 39121 p. 2). Because of the uncertainty in this parameter, as discussed in the previous paragraph, and consistent with the Agency's approach in making the low value (0.01) lower than the results obtained in DOE's analysis (0.08), the Agency selected a high value (0.60) that is higher than the highest value that has been interpreted from the TDEM data (0.55). The Agency has also considered the possibility that the WIPP-12 brine reservoir may underlie 100% of the site and therefore the probability of encountering pressurized brine would be 100%. This consideration is based on the assumption that the WIPP-12 reservoir is cylindrical in shape, which the Agency considers unlikely, and on the assumption that if present beneath the site, the reservoir is certain to yield sufficient brine to affect waste isolation, which the Agency considers unreasonable. Although the Agency agrees that part of the WIPP-12 reservoir may underlie part of the site, the TDEM data do not support speculation of a 100% probability of encounter. In view of the lack of support from the TDEM data and the other concerns expressed above, the Agency did not believe that an upper bound value higher than 0.60 was reasonable. The Agency also considered the possibility that the probability of encountering a brine reservoir would be zero. This possibility was also rejected based on the TDEM data which indicate the clear potential for a brine reservoir to lie beneath the site.

The sensitivity analysis showed that the CCDFs upon which regulatory compliance is based were not sensitive to changes ranging from the low to high value of this parameter (see SA Report 1998 Table 3.5-1). Despite a demonstrated low sensitivity, the Agency continued to disagree with DOE's technical approach for this parameter and based on the concerns expressed in public comments, the Agency required DOE to modify it in the PAVT by treating it as a sampled variable with a uniform distribution and a range of 0.01 to 0.60 (see Trovato 1997C Enclosure 2). A uniform distribution was mandated because the range of this parameter spans slightly more than an order of magnitude and the use of a uniform distribution will conservatively bias the sampling toward the high end. The range is the same as used in the SA and is based on the same rationale as described above for the SA. These changes increased the median value of this parameter from 0.08 to 0.305 and are expected to conservatively increase the frequency of encountering a Castile brine pocket in the PAVT.

4.2 2254 BOREHOLE - TAUFAIL: Waste Shear Resistance

The waste shear resistance is a measure of the resistance of the waste to erosion by moving borehole fluids at the waste-borehole interface. This parameter was used in the CUTTINGS_S code for calculating cavings releases. It was treated as a sampled value in the CCA PA with a uniform distribution and a range of 0.05 to 10.0 Pa. This range of values was derived by DOE from literature studies of erosion in San Francisco Bay mud and consideration of the mean particle size of the WIPP waste (see WPO # 40521 p. 18 and CCA, Volume XI, Appendix PAR p. PAR-117 [Docket: A-93-02, II-G-1]). This parameter represents the threshold value of fluid shear stress required to sustain general erosion of the borehole wall. Its value is considerably lower than and is not the same as the normal soil shear strength.

A similar parameter was independently assigned a quite different value by DOE in the spallings release calculations. That parameter was called the waste cementation strength. It is a measure of the resistance of the waste to erosion by moving pore gas and was assigned a constant value of 700 psi (6,895 Pa) (parameter BLOWOUT - CEMENT; see Section 3.1). Because both parameters are measures of resistance to erosion by moving fluids, the Agency considered that the basis for their assigned values should be correlated. The Agency's disposition of parameter BLOWOUT - CEMENT is described in Section 3.1. The parameter BOREHOLE - TAUFAIL has a significant influence on cavings releases and was therefore listed in Enclosure 3 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the waste shear resistance was studied in the Agency's SA using a low value of 0.01 Pa and a high value of 10 Pa (see SA Report 1998 Appendix PD Section PD-3.2). The low value was of most interest to the Agency because a weaker material would result in greater cavings releases. The low value was originally deemed unsupported but DOE provided additional erosional studies that suggested the minimum shear stress would actually be 0.1 Pa or greater. EPA accepted the 0.05 Pa as being acceptable because it is conservative. The high value was set at 10 Pa and is the same as the high end of the CCA range. The results of this analysis showed a sensitivity of 1413% to the change in this parameter, which the Agency considered to be significant (see SA Report 1998 Table 3.3-1). Because of its demonstrated sensitivity, the Agency required DOE to modify this parameter in the PAVT based on the results of the particle size distribution expert elicitation (see Trovato 1997C Enclosure 2 and Section 3.2 of this report).

DOE's proposal for estimating the value of parameter BOREHOLE - TAUFAIL based on the particle size distributions determined by the Expert Elicitation Panel (EEP) is summarized in a June 27, 1997 memorandum (WPO # 46646). The basis for convening such a panel for this parameter is discussed in Section 3.2 of this report. Based on the EEP results, the volume-averaged mean particle size for fully degraded waste was determined by DOE to range from a low of 0.1 cm to a high of 10 cm (assuming no cementation) or room-size (assuming cementation) (see WPO # 46936 and Section 3.2 of this report). The minimum value of 0.1 cm is much greater than the 40 microns used in the CCA spallings calculations. For conservatism, DOE based its estimate on the lower range of 0.1 to 10 cm and the minimum waste particle density of 2.5 gm/cm^3. DOE's approach used the Shield's parameter as mandated by the Agency (Trovato 1997C Enclosure 2), which relies on a measure of the central point of a population of particles of various sizes to determine the critical shear stress for an erodible, cohesionless sediment bed (Simon and Senturk 1992). Based on this approach, the DOE calculated critical shear stresses ranging from 0.64 Pa to 77 Pa. This range is higher than that used in the CCA PA and would lead to lower cavings releases. For conservatism, DOE proposed and the Agency accepted that the waste shear resistance in the PAVT be sampled from a log-uniform distribution with a range of 0.05 to 77 Pa. The log-uniform distribution was selected to provide equal weighting over the three orders of magnitude in the range. The low value was equal to the low end of the range used in the CCA, which DOE supported with additional information. This information indicated that very fine-grained materials are not cohesionless as assumed in the Agency's aforementioned Shields Parameter calculation. The information also showed that a lower bound of the critical shear stress for fine-grained, cohesive sediments is on the order of 0.05 Pa (Parthenaides and Paaswell 1970). The high end of the range was considered appropriate for cohesionless particles and was retained based on the EEP results.

4.3 3184 BH_SAND - PRMX_LOG: Long-Term Borehole Permeability

The long-term borehole permeability is the permeability assigned to an intrusion borehole when it is assumed to have been filled with casing corrosion products, plug degradation products, and native materials sloughed from overlying formations. DOE estimated the value of this parameter from a literature review using silty sand as a surrogate material (Freeze and Cherry 1979 Table 2.2). Because of its uncertainty, it was treated in the CCA as a sampled variable with a uniform distribution and a range of -14 to -11 log m^2. The Agency did not agree with the lower bound of this range and believes that the value may be may be closer to that of a borehole plug. The Agency was also not satisfied that DOE's range adequately captured the uncertainty of this parameter. This parameter has a potentially significant influence on long-term releases from intrusion boreholes and was listed in Enclosure 3 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the long term borehole permeability was studied in the Agency's SA using a low value of -17 log m^2 and a high value of -11 log m^2 (see SA Report 1997 Appendix PD Section PD-1.5). The low value was of most interest to the Agency because a less permeable material could result in greater gas pressure buildup in the repository with consequent increases in brine and spallings releases. It was selected based on the permeability of partially degraded concrete to reflect the possibility that the borehole plugs may not degrade as expected by DOE, but may instead remain as low-permeability barriers over the regulatory time frame. Information on the permeability of an intact borehole plug in salt obtained by DOE from field measurements at the WIPP Site and supporting laboratory tests was used by the Agency in determining this lower bound value (Christensen and Hunter 1980 Figure 4).

The upper bound of the permeability range was not changed in the sensitivity analysis because further reduction in this value would result in lower gas pressures and lower long-term releases. The analysis showed a 330% average change in the performance measures, which the Agency considered to be significant (see SA Report 1998 Table 3.1-1). Because of its demonstrated sensitivity, the Agency required DOE to treat this parameter (and its Y- and Z-direction counterparts) in the PAVT as a sampled variable with a uniform distribution and a range of -16.3 log m^2 to -11 log m^2 (see Trovato 1997B Enclosure 2 and Kruger 1997). The uniform distribution is the same as used in the CCA and was not changed. A uniform distribution was accepted for this logarithmic parameter because, based on present knowledge, the Agency believes that all values across the range of several orders of magnitude are equally likely. The lower bound of -16.3 log m^2 is the permeability assigned by DOE to an intact borehole plug (see Section 5.17 of this report). It was used by the Agency as the lower bound of this range because it approximates conditions that would occur if the plug degradation assumed by DOE in the PA did not occur. By selecting a low value of the sampled range based on the permeability of an undegraded plug, the analysis has the same type of impact as sampling an extended distribution of borehole plug lifetimes. Both analyses would include realizations with low plug permeabilities that constrain gas release through the borehole over long periods of time. For the same reasons as in the sensitivity analysis, the upper bound was allowed to remain the same as used in the CCA. Reducing the lower bound of this parameter was expected to result in conservatively higher repository gas pressures and higher radionuclide releases during inadvertent intrusions.

4.4 2918 CASTILER - VOLUME: Castile Brine Pocket Volume

The volume of a Castile brine pocket is a potentially important parameter related to the volume of brine that may be available to enter the repository, the rate of gas pressure buildup from waste corrosion and degradation, and the brine and spallings releases to the accessible environment. The parameter CASTILER - VOLUME was listed among the input parameters to the PA model and because considerably larger values for this parameter were available in DOE's supporting data, it was included in Enclosure 3 of the Agency's March 19, 1997 letter as requiring additional evaluation (Trovato 1997A). Upon further investigation, the Agency found that this parameter was not used by DOE in the 1996 CCA. Instead, the brine pocket volume was sampled from a predetermined range using the index parameter CASTILER - GRIDFLO and a porosity correction term (see SA Report 1998 Appendix PD Sections PD-1.9 and PD-1.10). Because it was not used in the CCA PA model, the parameter CASTILER - VOLUME was identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

As an alternative to this parameter and to achieve the same objective of incorporating larger brine pocket volumes, the Agency required DOE to modify the porosity correction terms in the PAVT. Because of the link between brine pocket volume and rock compressibility in determining the volume of brine that can be released from a brine pocket, and the simultaneous treatment of both parameters in the Agency's sensitivity analysis, this modification is discussed along with Castile brine pocket rock compressibility in Section 4.5 below.

4.5 61 CASTILER - COMP_RCK: Castile Brine Pocket Rock Compressibility

The Castile brine pocket rock compressibility is used along with other parameters in the PA model to calculate the volume of brine released from a Castile brine pocket. DOE estimated the value of this parameter based on a combination of field and literature data (see CCA Docket: A-93-02, II-G-1, Volume XI, Appendix PAR p. PAR-107 and WPO # 31084 p. 1). Because of its uncertainty, this parameter was treated as a sampled variable with a triangular distribution, a range of 5 E-12 Pa^{-1} to 1 E-8 Pa^{-1}, and a mode of 1 E-10 Pa^{-1}. Analysis by DOE subsequent to the CCA PA calculations suggested a different range, one that was more closely tied to field tests conducted in borehole WIPP-12 in a Castile brine reservoir on the WIPP Site (see WPO # 41887 pp. 1-3 and WPO # 44699 p. 1). Because of its relationship to the volume released from a brine reservoir, this parameter has a potentially significant influence on the volume of brine that may be available to enter the repository, the rate of gas pressure buildup from waste corrosion and degradation, and the brine and spallings releases to the accessible environment. This parameter was therefore listed in Enclosure 3 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the Castile brine pocket rock compressibility was studied in two different analyses conducted by the Agency. In the first of these sensitivity analyses, only the rock compressibility was varied to determine the sensitivity to variations in that parameter alone (see SA Report 1998 Appendix PD Section PD-1.8). In performing this first analysis, the compressibility was set at high and low values corresponding to the extremes of the range determined by DOE. During this analysis, the Castile brine pocket porosity was 0.0087, the parameter GRIDFLO was set at a median value of 16 corresponding to the CCA median brine pocket pore volume of 1.28 E+05 m^3, and all other sampled PA inputs were similarly fixed at their median values. The reservoir productivity ratio (pore volume times pore compressibility, or alternatively, pore volume times rock compressibility divided by porosity) corresponding to these values ranges from 7.4 E-05 to 1.5 E-01 m^3/Pa and is an estimate of the brine volume that the brine pocket is capable of releasing to an intrusion borehole per unit change in brine pocket pressure. These productivity ratios bracket the expected productivity ratio of approximately 4 E-02 m^3/Pa estimated for the brine reservoir encountered at WIPP-12 (based on a total pore volume of 2.7 E+06 m^3 [17 E+06 bbl] and a pore compressibility of 1.45 E-08/Pa [100 E-06/psi]; see WPO # 42085 p. H-53). This sensitivity analysis is therefore also considered by the Agency to provide a test of the sensitivity of PA model results to changes in the volume of brine released by a Castile brine pocket. The Agency considers the WIPP-12 reservoir to provide an appropriately conservative reference value for reservoir properties because of its relatively large size and its proximity to the WIPP Site. Although the compressibility and therefore the reservoir productivity ratio variation ranged over nearly four orders of magnitude in the sensitivity analysis, the average change in the performance measures was only 2% and was not considered to be significant (see SA Report 1998 Table 3.1-1).

In the second of these sensitivity analyses, the compressibility was varied along with the porosity correction term to effect a significant increase in the brine pocket volume (see SA Report 1998 Appendix PD Section PD-1.10). In this analysis the porosity correction term was assigned a low value of 0.1848, corresponding to a brine pocket pore volume of 3.4 E+06 m^3, and a high value of 0.924, corresponding to a brine pocket pore volume of 1.7 E+07 m^3 (see SA Report 1998 Appendix PD Section PD-1.10 for additional information on this analysis and an explanation of the relationship between this correction term and the brine pocket pore volume). This brine pocket volume range was suggested by DOE based on an analysis of the WIPP-12 brine pocket and is considered by the Agency to provide a reasonable estimate of the possible range of volumes that may be present at the site (see WPO # 41887). In this second sensitivity analysis the productivity ratio ranged from 7.8 E-03 to 2.0 E-01 m^3/Pa and also bracketed the aforementioned WIPP-12 productivity ratio. Again, the average change in the performance measures was low, only 1%, and was not considered significant.

Even though the sensitivity of the PA model to changes in rock compressibility and brine pocket volume was found to be low, the Agency was not satisfied with DOE's technical justification for the brine pocket rock compressibility and pore volume range used in the CCA PA and because of numerous public comments the Agency required DOE to change those ranges in the PAVT (Trovato 1997B Enclosure 2). In the Agency's letter, the DOE was required to treat the rock compressibility as a sampled variable with a triangular distribution, a revised range of 2 E-11 Pa^{-1} to 1 E-10 Pa^{-1}, and a revised mode of 4 E-11 Pa^{-1}. This revised range was estimated by DOE and accepted by the Agency based on an analysis of the Castile brine pocket encountered in borehole WIPP-12 (WPO # 41887). As previously mentioned, the Agency considered the WIPP-12 reservoir to provide appropriately conservative reference values for Castile brine reservoir properties and therefore considered this analysis to be appropriate and the results preferable to data taken from other formations at WIPP or from non-WIPP sources reported in the literature. The form of the distribution was not changed and remained the same as in the CCA. The Agency concurred with the form of the distribution selected by DOE because, although a simple form was warranted because little was known about the distribution's specific shape, the Agency agreed that midrange values were more likely than the extreme bounding values.

Although not documented in the aforementioned Agency letter, the Agency also requested the DOE to change the porosity correction term in the PAVT to a sampled variable with a triangular distribution, a range of 0.1848 to 0.9240, and a mode of 0.3696. A new parameter (8000 CASTILER - POR_BPKT) was created in the PA model to allow the porosity correction term to be sampled. The triangular distribution reflects the Agency's belief that an intermediate value is more likely that either extreme value, yet it retains a simple shape that reflects the uncertainty about the distribution's specific shape. The mode is equivalent to a brine pocket pore volume of 6.8 E+06 m^3 and is equal to the average of the range of WIPP-12 brine pocket volumes estimated by Popielak et al. (1.7 E+06 to 8.7 E+07 bbl; see WPO # 42085 p. H-60). The range was determined from a reanalysis of the WIPP-12 data. It is higher than the range of Popielak et al. and is the same as used in the aforementioned second sensitivity analysis (see WPO # 41887). The productivity ratio for the PAVT has the same range as for the second sensitivity analysis (7.8 E-03 to 2.0 E-01 m^3/Pa) and brackets the WIPP-12 productivity ratio of 4 E-02 m^3/Pa. These changes have the effect of modeling the characteristics of Castile brine pockets in the PAVT after those of the WIPP-12 brine reservoir. The parameter changes in the PAVT reduced the rock compressibility range and mode to more appropriate values and increased the brine reservoir volume. The reduced compressibility would tend to reduce the reservoir's capability to release brine, while the increased volume would tend to increase that capability. Because the volume increase was substantially greater than the compressibility reduction, the net effect is expected to conservatively increase the volume of brine available to flow from the reservoir.

5.0 PARAMETERS WITH QUESTIONABLE VALUES OR RANGES

Parameters for which the Agency has reviewed the supporting information and has questions about the values selected are addressed in this section. These parameters are listed in Enclosure 4 of the Agency's March 19, 1997 letter (Trovato 1997A). Each of the following subsection headings identifies the parameter's number, Material ID and Parameter ID, followed by a brief description of the parameter.

5.1 27 BOREHOLE - DOMEGA: Drill String Angular Velocity

This parameter is the rotational velocity of the drill string in an intrusion borehole. It is used in calculating cavings release volumes in the CUTTINGS_S code. This parameter is treated as a constant in the CCA and is equal to the median of a constructed cumulative distribution of rotational velocities used in current practice when drilling through salt (7.8 radians per second; see WPO # 31512 p. 2 and WPO # 37765 p. 49). In its parameter review, the Agency found that the range of angular velocities used in salt was large, ranging from 4.2 to 23 radians per second (A-93-02, II-G-1, Volume V, Appendix Cuttings, Section 2.3). Because of the potential importance of this parameter in calculating cavings releases and the magnitude of the range, the Agency questioned the use of a single value rather than a range in the CCA and listed this parameter in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to drill string angular velocity was tested by the Agency by assigning low and high values equal to the extremes of the aforementioned range identified by DOE (see A-93-02, II-G-1, Volume V, Appendix Cuttings, Section 2.3 and SA Report 1998 Appendix PD Section PD-3.1). The results of the analysis showed a 60% change in the cavings releases, which the Agency found to be potentially significant. In view of this demonstrated sensitivity and the potential importance of cavings releases in meeting the Agency's regulatory criteria, the DOE was required by the Agency's April 25, 1997 letter to treat the drill string angular velocity as a sampled variable in the PAVT with a constructed cumulative distribution, a minimum of 4.2 radians/second, a maximum of 23 radians/second, and a median of 7.77 radians/second (Trovato 1997C Enclosure 2). A constructed cumulative distribution is a distribution based directly on original data. It was selected because sufficient data were available to support this approach. This range is the same as used in the SA and was considered appropriate by the Agency because, as described above, it is based on an acceptable study of current drilling practices in salt. These changes are expected to conservatively increase the range of cavings releases in the PAVT.

5.2 64 CASTILER - POROSITY: Castile Brine Pocket Porosity

The effective porosity of a Castile brine pocket is one of the parameters used in the BRAGFLO code to calculate the brine pocket volume. Although this parameter is identified in the PA database as a sampled variable with a Student T distribution, a minimum of 0.002, a maximum of 0.016, and a median of 0.0087, it is treated as a constant equal to the median value of 0.0087 in the CCA. These values are based on the results of three laboratory measurements of effective porosity performed on intact pieces of Castile anhydrite core (see WPO # 42085). The documentation further stated that the porosity value used in the model was calculated by multiplying the value of this parameter by the number of brine pockets, and dividing that product by 5 (see WPO # 40434). Because the purpose of this calculation was not understood and its justification was not available at the time of the initial review, the Agency included this parameter in Enclosure 4 of its March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

In subsequent reviews, the Agency learned that the aforementioned calculation was associated with DOE's assumption that brine pockets occur beneath the WIPP Site in five discrete sizes with constant pore volume increments of 32,000 m^3 and total pore volumes ranging from 32,000 to 160,000 m^3 (see the SA Report 1998 Appendix PD Section PD-9 for additional discussion of this approach). Although at first confusing , the Agency found this approach to be internally consistent and acceptable. This parameter was therefore identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.3 66 CASTILER - PRESSURE: Castile Brine Pocket Pore Pressure

This parameter is the undisturbed brine pressure in a Castile brine pocket before intrusion by an exploration borehole. It was estimated by DOE based on available information on pressures in brine pockets encountered in the Delaware Basin (see CCA Docket: A-93-02, II-G-1, Volume XI, Appendix PAR p. PAR-101, WPO # 37148 p. 1, and WPO # 37973 pp. 1-3). Because of its relatively high uncertainty, this parameter was treated as a sampled variable in the CCA with a triangular distribution, a range of 1.11 E+07 Pa to 1.70 E+07 Pa, and a median of 1.27 E+07 Pa. Although the basis for selecting the range of pressures used in the CCA was well documented, the Agency found that the form of the distribution was insufficiently explained. Because of the potential importance of this parameter in calculating the brine volume in the repository and the Agency's questions regarding the distribution used in the CCA, it was listed in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to the Castile brine pocket pore pressure was tested by the Agency by assigning low and high values equal to the extremes of the aforementioned range identified by DOE (see SA Report 1998 Appendix PD Section PD-1.11). The results of the analysis showed no model sensitivity (see SA Report 1998 Table 3.1-1). In view of this lack of sensitivity, the DOE was informed in the Agency's April 25, 1997 letter that this parameter was no longer in question (Trovato 1997C Enclosure 1).

5.4 259 PAN_SEAL - PRMX_LOG: Panel Seal Permeability

This parameter is the permeability of the concrete and crushed salt seals used to isolate the waste panels after they have been filled. The panel seal permeability was assigned by DOE to be the same as that of the DRZ. Although the seal permeability would be expected to change over time as the concrete degraded and the halite was compressed by creep closure, it was treated as a constant in the CCA equal to -15 log m^2. The uncertainty in this parameter led the Agency to question the DOE's approach. Because of the potential importance of this parameter in restricting brine movement within the repository and the Agency's questions regarding the value used in the CCA, it was listed in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to the panel seal permeability was tested by the Agency by determining the impact of low and high parameter values on PA performance measures. The effect of a reduction in the CCA value was of primary interest to the Agency because it would restrict gas flow within the repository. The effect of an increase in the CCA value was also of interest because it would allow brine to move more freely within the repository. In performing the SA, the Agency used a low value of -21 log m^2 and a high value of -13 log m^2. Selecting a low value that is six orders of magnitude less than the CCA value and a high value that is two orders of magnitude greater than the CCA value was considered to provide an adequate analysis of sensitivity (see SA Report 1998 Section 1.14). The results of the analysis showed no model sensitivity (see SA Report 1998 Table 3.1-1). In view of this lack of sensitivity, the DOE was informed in the Agency's April 17, 1997 letter that this parameter was no longer in question (Trovato 1997B Enclosure 1).

5.5 528 S_ANH_AB - POROSITY: Effective Porosity of Anhydrite Beds A and B

This parameter is the initial effective porosity of anhydrite beds A and B. Its value was determined by DOE as the mean porosity of 16 field samples (see WPO # 34860 p. 2). This parameter was treated as a constant in the CCA equal to 0.011. Because of its potential importance in calculating actinide transport rates to the accessible environment, the Agency questioned the sensitivity of the PA code to the extreme porosity values found in the field samples. Because of this uncertainty, the Agency listed this parameter in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the anhydrite effective porosity value was tested as part of the Agency's sensitivity analysis. In performing this analysis, the effective porosity of all anhydrite beds was assigned a low value of 0.006 and a high value of 0.017 based on the extreme porosity values measured in the aforementioned field samples. (see SA Report 1998 Appendix PD Section PD-1.2). The results of the analysis showed no model sensitivity (see SA Report 1998 Table 3.1-1). In view of this lack of sensitivity, the DOE was informed in the Agency's April 17, 1997 letter that this parameter was no longer in question (Trovato 1997B Enclosure 1).

5.6 567 S_MB138 - POROSITY: Effective Porosity of Anhydrite Marker Bed 138

This parameter is the initial effective porosity of anhydrite Marker Bed 138. Its was assigned the same constant value by DOE as the effective porosity of anhydrite beds A and B discussed in Section 5.5 above, and consequently carried the same Agency concerns. Because of these concerns, the Agency listed this parameter in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A). The sensitivity of the PA model to changes in the value of this parameter was tested by the Agency in the same analysis as the effective porosity for beds A and B. The same low and high values were assigned as described in Section 5.5, and no model sensitivity was found (see SA Report 1998 Table 3.1-1). In view of this lack of sensitivity, the DOE was informed in the Agency's April 17, 1997 letter that this parameter was no longer in question (Trovato 1997B Enclosure 1).

5.7 588 S_MB139 - POROSITY: Effective Porosity of Anhydrite Marker Bed 139

This parameter is the initial effective porosity of anhydrite Marker Bed 139. Its was assigned the same constant value by DOE as the effective porosities of anhydrite beds A and B and Marker Bed 138 discussed in Sections 5.5 and 5.6 above, and consequently carried the same Agency concerns. Because of these concerns, the Agency listed this parameter in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A). The sensitivity of the PA model to changes in the value of this parameter was tested by the Agency in the same analysis as the effective porosity for the other anhydrite beds. The same low and high values were assigned as described in Section 5.5, and no model sensitivity was found (see SA Report 1998 Table 3.1-1). In view of this lack of sensitivity, the DOE was informed in the Agency's April 17, 1997 letter that this parameter was no longer in question (Trovato 1997B Enclosure 1).

5.8 651 WAS_AREA - ABSROUGH: Waste Area Absolute Roughness

This parameter is a measure of the roughness of the wall of an intrusion borehole where it passes through the waste. It was listed by DOE as an input to the CUTTINGS_S model for use in calculating cavings releases. Because the value of this parameter was poorly documented and the cavings volume was an important contributor to overall releases, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A). Upon further investigation, it was found that this parameter was not used by DOE in the 1996 CCA PA model to set the absolute roughness of the waste and had no effect on the model results. This parameter was therefore identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.9 653 WAS_AREA - COMP_RCK: Waste Area Rock Compressibility

This parameter is the compressibility of the waste material in the repository. DOE assigned a zero value to this parameter in the CCA and noted that the compressibility of the waste is addressed in the porosity surface room closure calculations (see CCA Docket: A-93-02, II-G-1, Volume I, Chapter 6, p. 6-101). Because this parameter was not well documented in the DOE's data base and the Agency questioned the use of a zero value by DOE, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the waste area rock compressibility was studied in the Agency's SA. A range for waste compressibility was calculated by the Agency based on waste strength information presented in the 1992 Draft Performance Assessment (SNL 1992 Vol

3 p. 2-69). Upon further investigation, it was found that although this parameter was retained by DOE in the 1996 CCA PA model, it was not actually used in the calculations and its value had no effect on the model results. This parameter was therefore identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.10 1992 WAS_AREA - DIRNCCHW: Bulk Density of Iron Containers for CH Waste

This parameter is the average bulk density of iron containers for contact-handled waste at WIPP. It was used in the CCA to calculate the contribution of the iron containers themselves to the total mass of iron available for corrosion in the repository. The value of this parameter was determined by DOE from information in the Baseline Inventory Report (BIR), which documents the physical characteristics of the waste containers expected to be received by the WIPP (WPO # 32328). The total mass of iron in the repository is used along with brine inflow and other parameters to calculate gas generation rates and repository gas pressures, which have been found to be important drivers for brine and spallings releases. Because this parameter is potentially important in repository performance calculations and adequate documentation was not found in the Agency's initial review, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

Upon completing a comprehensive evaluation of the BIR (EPA 1998a), the Agency confirmed that the necessary supporting information for this parameter was appropriately documented and that the related uncertainty was low. This parameter was therefore identified in the Agency's letter of April 17, 1997 as being no longer in question (Trovato 1997B Enclosure 1).

5.11 1993 WAS_AREA - DIRNCRHW: Bulk Density of Iron Containers in RH Waste

This parameter is the average bulk density of iron containers for remote-handled waste at WIPP. It was used in the CCA to calculate the contribution of the iron containers themselves to the total mass of iron available for corrosion in the repository. The value of this parameter was determined by DOE from information in the Baseline Inventory Report (BIR), as discussed in Section 5.10 for the parallel parameter for contact-handled waste (WPO # 32328). Because this parameter is potentially important in repository performance calculations and adequate documentation was not found in the Agency's initial review, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

Upon completing a comprehensive evaluation of the BIR (EPA 1998a), the Agency confirmed that the necessary supporting information for this parameter was appropriately documented and that the related uncertainty was low. This parameter was therefore identified in the Agency's letter of April 17, 1997 as being no longer in question (Trovato 1997B Enclosure 1).

5.12 2040 WAS_AREA - DIRNCHW: Average Density of Iron-Based Material in CH Waste

This parameter is the average density of iron-based material in contact-handled waste at WIPP. Its value was determined by DOE from information in the Baseline Inventory Report (BIR), which documents the physical characteristics of the wastes expected to be received at WIPP (WPO # 32328). It was used by DOE to determine the mass of iron-based material in the waste. Because this parameter appeared potentially important in repository performance calculations and adequate documentation was not found in the Agency's initial review, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in waste density was studied in five analyses performed by the Agency. These studies were performed by determining the change in model performance measures resulting from varying the average density of iron-based waste materials, cellulosics, rubber, and plastics in the waste. The values of each of these densities were changed both separately and collectively, and the results are described in the Agency's SA Report (1997 Section 3.1). The average bulk densities of iron containers was not varied in these analyses because their uncertainty is low. The average changes of the PA performance measures due to changes in waste density parameters were found to be greater than for any other parameter studied, and ranged from about 70,000% to 104,000%. The high sensitivity of the repository performance measures to changes in waste density (or to the calculated mass of waste in the repository) was not unexpected because the SA was conducted assuming that all waste received was either the maximum or the minimum density. However, it should be noted that because waste density was an input to the BRAGFLO code, the Agency's performance measures were a series of key outputs such as repository gas pressures and repository brine flows that are calculated by BRAGFLO, rather than direct releases to the accessible environment that are not calculated by BRAGFLO. The selection of performance measures for the SA is more fully discussed in Appendix PM of the SA Report (1997).

Because of the high sensitivity to changes in waste density, the approach taken by DOE in determining density data for the CCA PA was reviewed by the Agency in detail (EPA 1998a). The average densities for all waste types were found to be appropriately calculated from data presented in the BIR (WPO#32328), and account for the expected waste inventory. The Agency considered the minimum and maximum densities presented by the generator sites in Appendix BIR, Appendix P (A-93-02, II-G-1, Volume III-V, Appendix BIR) of the CCA and determined that use of the lowest and highest minimum and maximum values in PA would not be a realistic representation of the expected inventory. For example, although one generator site identified a minimum density of 0 for a parameter in a site-specific waste stream, it would be inappropriate to apply this value to all similar WIPP waste streams, or to use this as a representative minimum value for the parameter.

EPA examined the average values provided by generator sites on a site-specific waste stream basis and also on an average basis across all WIPP waste streams. The Agency found that use of the average value for waste densities provides a realistic and justifiable representation of the expected waste inventory. The density parameters were therefore identified in the Agency's letter of April 17, 1997 as being no longer in question (Trovato 1997B Enclosure 1).

5.13 2041 WAS_AREA - DCELLCHW: Average Density of Cellulosics in CH Waste

This parameter is the average density of cellulosics in contact-handled waste at WIPP. Its value was determined by DOE from information in the Baseline Inventory Report (BIR), which documents the physical characteristics of the wastes expected to be received at WIPP (WPO # 32328). It was used by DOE to determine the mass of cellulosic materials in the repository. This parameter was included along with other waste density parameters in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A). Upon evaluating this parameter in detail, the Agency reached the same conclusions as discussed in Section 5.12 above. Although PA modeling results were found to be sensitive to its value, for the reasons given in Section 5.12 this parameter was identified to the DOE in the Agency's letter of April 17, 1997 as being no longer in question (Trovato 1997B Enclosure 1).

5.14 2274 WAS_AREA - DCELLRHW: Average Density of Cellulosics in RH Waste

This parameter is the average density of cellulosics in remote-handled waste at WIPP. Its value was determined by DOE from information in the Baseline Inventory Report (BIR), which documents the physical characteristics of the wastes expected to be received at WIPP (WPO # 32328). It was used by DOE to determine the mass of cellulosic materials in the repository. This parameter was included along with other waste density parameters in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A). Upon evaluating this parameter in detail, the Agency reached the same conclusions as discussed in Section 5.12 above. Although PA modeling results were found to be sensitive to its value, for the reasons given in Section 5.12 this parameter was identified to the DOE in the Agency's letter of April 17, 1997 as being no longer in question (Trovato 1997B Enclosure 1).

5.15 2907 STEEL - CORRMCO2: Steel Corrosion Rate

This parameter is the rate of steel corrosion in a brine-saturated repository without CO_2 present in the brine. Use of this parameter assumes the presence and complete effectiveness of the MgO backfill in reacting with and removing the CO_2 from solution. The steel corrosion rate was estimated by DOE based on long-term anoxic steel corrosion experiments (see CCA Docket: A-93-02, II-G-1, Volume XI, Appendix PAR p. PAR-15). Because of its uncertainty, this parameter was treated as a sampled variable in the CCA with a uniform distribution, a range from zero to 1.59 E-14 m/s, and a median of 7.94 E-15 (see WPO #35162 p. 5 and WPO #35181 p. 1, both in WPO #30819). Because the Agency questioned both the lower and upper bounds for this parameter, it was included along with other waste density parameters in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the steel corrosion rate was studied in the Agency's SA. Based on a review of the experimental corrosion data, the Agency agreed that under some circumstances the rate of corrosion could be very low but may not be zero. The Agency's objective in the sensitivity analysis was to determine the effect of a non-zero lower bound to the corrosion rate, and accordingly increased the lower bound to 1 E-30 m/s to check the sensitivity to a small but nonzero value. The baseline and high values remained equal to those used by DOE in the CCA. Although the results indicated that the performance measures were not sensitive to this change in the lower bound (an average change of 7% was found; see SA Report 1997 Table 3.1-1), the upper bound remained in question and was found in DOE's experimental results to be potentially sensitive to several aspects of the repository environment..

The effect of contact with salt on corrosion rates was evaluated in DOE tests. A DOE test in which steel was embedded in a bentonite-crushed salt mixture yielded a corrosion rate approximately double the rate with no bentonite present (Telander and Westerman 1997 p. 6-39). However, a similar test conducted without bentonite present showed no rate increase (5 and Westerman 1995 p. 6-43). The WIPP design presented in the CCA does not include a bentonite backfill and based on the foregoing experimental results, the Agency does not consider contact with salt alone to significantly affect corrosion rates.

The Agency considers DOE's use of long-term test results to be appropriate considering that the corrosion rate parameter is intended to reflect repository behavior over 10,000 years. Isolated local conditions that may result in higher short-term corrosion rates would have little impact on overall, long-term repository conditions. DOE's experiments were conducted under a pH of 9.5 to 10, which represents the lowest pH that would occur in the repository in the presence of an MgO backfill that sequesters CO_2 from solution (see Wang and Brush 1996 p. 5). Although a local, lower pH environment could result in higher corrosion rates, based on the findings of the DOE's independent Conceptual Models Peer Review Panel (Wilson et al. 1997B p. 12ff) and the Agency's own review, the MgO backfill is expected to be effective in controlling pH.

An average corrosion rate of 2.25 E-14 m/s was determined by DOE from the average hydrogen gas generation between the 12th and 24th months of a test in a sealed chamber where the steel specimens were immersed in brine and over-pressured with nitrogen at a maximum end-of-test pressure of 17 atm. To obtain the maximum CCA value, this rate was adjusted downward by a factor of 70% based on another test of 38.5 months duration where a small amount of CO_2 was added to the nitrogen cover gas (Telander and Westerman 1995). However, other experiments of six months duration conducted with a hydrogen cover gas indicated that the corrosion rate first decreased at overpressures from 2 to 70 atm and then increased at overpressures from 70 to 127 atm (lithostatic pressure at the repository horizon is about 150 atm). An additional test with a nitrogen cover gas produced a corrosion rate about twice as high as a companion test at 10 atm. Because the repository pressure may, under some circumstances, approach or exceed lithostatic and because the experimental corrosion rates increase at these higher pressures, in the Agency's letter of April 17, 1997 (Trovato 1997B Enclosure 2) the DOE was required to double the upper bound in the PAVT to 3.17 E-14 m/s to reflect the effect of factors such as increased pressure on the rate. A greater increase in the upper bound was not supported by available data. Higher corrosion rates are expected to have a conservative influence on repository performance because they result in increased rates of gas generation. At longer times, the effect of an increased corrosion rate is expected to be reduced because of limited brine availability.

The DOE's experimental results also indicated that when aluminum is present the steel corrosion rate increased markedly during the first 13 months of a test but then remained constant for the next 11 months (Telander and Westerman 1995). Telander and Westerman concluded that the corrosion enhancement did not appear, on the basis of the limited tests performed, to be a long-lived effect. The Agency believes that this position is reasonable, but notes that the increased rate used in the PAVT is reflective of such a possibility.

The Agency did not change the lower bound of zero used by DOE in the CCA. Although the Agency does not expect the rate to drop to identically zero, it could drop to a low value; however, the Agency's sensitivity analysis showed that such a change would have no significant impact on PA modeling results and would not be necessary in the PAVT. The Agency did not change the uniform distribution used by DOE in the CCA because this parameter spans several orders of magnitude and sampling from such a distribution conservatively favors higher corrosion rates.

5.16 3147 CONC_PLG - POROSITY: Borehole Plug Porosity

This parameter is the effective porosity assigned to a concrete plug expected to be placed by drillers when sealing an intrusion borehole. DOE estimated borehole plug porosity from engineering data on field-emplaced concrete structures. Concrete porosities were estimated to range from 25% to 40%, with a median value of 32% (CCA Docket: A-93-02, II-G-1, Volume X Appendix MASS Attachment 16-3 p. D-2 and Figure C-1). This parameter was treated as a constant by DOE in the CCA PA equal to 0.32. The Agency questioned the use of a constant value for this parameter in light of the ranges provided for it in the literature and also in view of its potential importance in determining transport rates through plugged boreholes. Because of these concerns, this parameter was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the borehole plug porosity was studied in the Agency's SA. A range for this parameter of 0.24 to 0.40 was determined by the Agency based on the aforementioned literature information. The results of the analysis showed no sensitivity of the performance measures to these changes, and this parameter was therefore identified in the Agency's letter of April 17, 1997 as being no longer in question (Trovato 1997B Enclosure 1).

5.17 3185 CONC_PLG - PRMX_LOG: Borehole Plug Permeability

This parameter is the permeability assigned to a concrete plug expected to be placed by drillers when sealing an intrusion borehole and is effective for 200 years in the CCA PA calculations. DOE estimated borehole plug permeability through direct measurement of the permeability of a concrete borehole plug at the WIPP Site (Christensen and Hunter 1980 Figure 4). This parameter was treated as a constant in the CCA equal to -16.3 log m^2 (see CCA Docket: A-93-02, II-G-1, Volume X, Appendix MASS Attachment 16-3 p. 12). The Agency questioned the use of a constant value for this parameter in view of its potential importance in determining gas and brine flow rates through plugged boreholes and was included it in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the borehole plug permeability was studied in the

Agency's SA by determining the variation in model performance measures to changes in the value of this parameter. The high end of the range (-11 log m^2) was determined by the Agency based on the high end of the range of degraded plug permeabilities estimated by DOE (see CCA Docket: A-93-02, II-G-1, Volume X, Appendix MASS Attachment 16-3 p. 14). The low end of the range (-18 log m^2) is the lowest value measured for the aforementioned WIPP borehole plug grout in laboratory tests (Christensen and Hunter 1980 p. 4). The results indicated a 101% average change in the performance measures to these changes in the parameter value, which the Agency considered to be significant. The DOE was therefore required by the Agency's letter of April 17, 1997 (Trovato 1997B Enclosure 2) to treat this parameter as a sampled value in the PAVT with a uniform distribution, a lower bound of -19 log m^2, and an upper bound of -17 log m^2. A uniform distribution for the logarithmic values was selected to provide equal weight across the range of this parameter. The lower bound is one order of magnitude lower than the lowest value measured for the WIPP borehole plug grout in the aforementioned laboratory tests. This is considered to be a more conservative lower bound because a less permeable borehole plug may result in higher repository gas pressures and greater releases during subsequent exploratory drilling intrusions. The upper bound is equal to the upper bound assumed for concrete in the shaft seals. It is based on the high end of the range of values from laboratory measurements, as adjusted upward to account for uncertainties in field placement techniques and minor concrete deterioration (see WPO # 30640 Section III Vol. 3 Part 2.2.1 p. 1). DOE was also mandated to change the Y- and Z-direction counterparts of this permeability in the same manner.

5.18 3256 BLOWOUT - FGE: Gravity Scaling Factor

The gravity scaling factor is an experimentally determined parameter used by DOE in the CUTTINGS_S code to relate the limiting fracture erosion velocity to the effects of gravity in calculating spallings release volumes. It is one of three factors applied by DOE to forces resisting waste erosion during a spallings event. These forces were the gravitational forces on the particle, capillary forces resulting from partial brine saturation, and the binding forces of particle cementation. The first two of these scaling factors were empirically determined from experimental results. The gravity scaling factor was determined to equal 18.1 and the capillary scaling factor was determined to equal zero (see WPO #35695 p. 32 and Lenke et al. 1996 p. 27). The third factor, the cementation scaling factor, is discussed in Section 3.1 of this report. The Agency questioned the applicability of the experimental results to spallings releases under WIPP repository conditions, and considered this parameter to be potentially important because of its use in directly calculating a release from the repository. Because of these concerns, this parameter was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

Subsequent to the aforementioned letter, the DOE proposed and the Agency accepted a change in the way that spallings releases would be addressed in the PAVT that eliminated the need for this parameter. This change is discussed in Section 3.1 of this report.

5.19 3259 BLOWOUT - APORO: Waste Permeability in CUTTINGS_S Model (663 WAS_AREA - PRMX_LOG)

(2131 REPOSIT - PRMX_LOG)

Waste permeability was identified by DOE as the input parameter BLOWOUT - APORO to the CUTTINGS_S model in the model documentation (see WPO #40521 p. 38). This parameter was treated as a constant in the CCA with a value of 1.7 E-13 m^2. The Agency questioned this parameter because of its potential importance in calculating a direct waste release to the ground surface. It was therefore included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

DOE was subsequently required by the Agency's letter of April 25, 1997 (Trovato 1997C Enclosure 2) to change the value of this parameter in the PAVT to 2.4 E-13 m^2. This parameter value is based on a recalculation of the weighted sum of the permeabilities of the individual waste components using the expected value of a piecewise-linear cumulative distribution rather than a uniform distribution (see CCA Docket: A-93-02, II-G-1, Volume XII, Appendix PEER p. 5-14). The Agency considers this change to be minor; it was made primarily to correct a computational error rather than to modify a concept. The Agency did not require this parameter to be treated as a sampled variable based on the reasoning of the DOE's Engineered Systems Data Qualification Peer Review Panel. The waste permeability, as corrected, was found by that panel to be not unreasonable when compared with permeabilities of compacted waste in municipal landfills (CCA Docket: A-93-02, II-G-1, Volume XII, Appendix PEER p. 5-18). Also, although that Panel estimated that uncertainties could cause the waste permeability to vary by up to an order of magnitude (CCA Docket: A-93-02, II-G-1, Volume XII, Appendix PEER Attachment PEER-5 p. 5-17), the Agency concluded that because the waste permeability is already more than two orders of magnitude higher than the permeability of any other geologic or seal component, flow through the waste would be relatively fast and long term releases to the accessible environment would be fairly insensitive to changes in waste permeability within an order of magnitude. Although direct brine releases during drilling intrusions would change in proportion to the changes in waste permeability, these releases constitute a small fraction of the total radionuclide releases from the repository and changes in their value would not significantly affect the mean total release (see CCA Volume I Figure 6-41).
Upon further review, the Agency found that despite the identification of this parameter as an input to CUTTINGS_S, it was not used in the final CCA version of that model. Instead, the waste permeability was incorporated using parameters 663 (WAS_AREA - PRMX_LOG) and 2131 (REPOSIT - PRMX_LOG). Both of these parameters were given constant values of 1.7 E-13 m^2 in the CCA. DOE was therefore informed that parameters 663 and 2131 must be changed in the PAVT to 2.4 E-13 m^2 in the X-, Y-, and Z-directions (see Kruger 1997). This is the value listed for parameter BLOWOUT - APORO in the Agency's letter of April 25, 1997 (Trovato 1997C Enclosure 2).

5.20 3429 PHUMOX3 - PHUMCIM: Humic Colloid Proportionality Constant in Castile Brine

This parameter is the proportionality constant for sorption of +3 actinides to humic colloids in Castile brine. It is defined as the ratio of the moles of actinide sorbed on humic colloids to the moles of actinide remaining in solution. Actinides with an oxidation state of +3 predominate the mobile radionuclide inventory and are the most important in evaluating releases. Although only the proportionality constant for actinides with an oxidation state of +3 in Castile brine is addressed here, DOE also assigned proportionality constants for actinides with other oxidation states and for actinides in Salado brine. The humic colloid proportionality constants were determined by DOE largely through literature reviews. These values were assigned to oxidation states and brine types independent of element type because sorption to large humic molecules occurs through chemical complexation and is more sensitive to oxidation state and the chemical environment of the brine than to the specific actinide elements present. Because of its potential importance and uncertainty, DOE treated parameter PHUMOX3 - PHUMCIM as a sampled variable in the CCA with a cumulative distribution, a range of 0.065 to 1.6, and a median of 1.37. The Agency considered this parameter to be potentially important in computing brine releases and included it in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the humic colloid proportionality constant was studied by the Agency in two sensitivity analyses. In the first of these analyses, the values of this constant were simultaneously changed along with the values of other parameters associated with actinide solubility (see SA Report 1997 Appendix PD Section PD-4.1). In the second analysis, the values of this constant were varied alone (see SA Report 1997 Appendix PD Section PD-4.3). In both analyses, the humic colloid proportionality constants were changed simultaneously for all actinide oxidation states and for both Castile and Salado brines. The ranges used in the sensitivity analysis were taken from the extremes of the ranges provided in DOE's documentation, and were considered by the Agency to be adequate for testing sensitivity (see WPO #42248 Table A and SA Report 1997 Appendix PD Sections PD-4.1 and PD-4.3). The results of these analyses are summarized in the SA Report (1997 Table 3.4-1). Although an average 51% change in the performance measures was found in the first analysis when solubilities were also changed, only a 3% change was found in the second analysis when only the humic colloid proportionality constants were changed. This indicates that the humic colloid proportionality constants were not the primary source of the 51% change in the first analysis, and that the PA results are not sensitive to changes in these parameters. Because of a low sensitivity, this parameter was therefore identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.21 3471 BLOWOUT - MAXFLOW: Maximum Period of Uncontrolled Borehole Flow

This parameter defines the maximum time period during which uncontrolled brine and gas flow is assumed to occur from an exploration borehole that intrudes the repository. The value of this parameter was set at 11 days by DOE based on the time that was required to control the problematic South Culebra Bluff Unit 1 well in January 1978 (see WPO #40520 p. 198 and WPO #43672 p. 10). The effort to control this well is considered by DOE to be a good analog to a hypothetical extreme loss of control during exploratory drilling at the WIPP Site because of its proximity to WIPP, the similarity of geology, and the time required to mobilize the resources and expertise to control the well (see Boak et al. 1996 p. A-6). The Agency questioned the value of this parameter because of the small information base from which it was drawn and because of its potential importance in determining the magnitude of a direct brine release. This parameter was therefore included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the maximum period of uncontrolled borehole flow was evaluated in the Agency's SA by determining the change in the performance measure for high and low values of this parameter. The low value selected by the Agency was 5 days and is equal to the high end of the range for the minimum period of uncontrolled borehole flow (see Section 5.22 of this report). The high end is equal to 20 days. This value is nearly double the DOE value and was considered by the Agency to provide an adequate test of sensitivity. The results showed a change in the performance measure of 197%. Although this sensitivity was considered by the Agency to be significant, upon further evaluation of DOE's documentation of drilling histories in the Delaware Basin, the Agency concluded that DOE's selection of 11 days as an upper limit for uncontrolled borehole flow was appropriate because of the close analogies that can be made to drilling at the WIPP Site. This parameter was therefore identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.22 3472 BLOWOUT - MINFLOW: Minimum Period of Uncontrolled Borehole Flow

This parameter defines the minimum time period during which uncontrolled brine and gas flow is assumed to occur from an exploration borehole that intrudes the repository. The value of this parameter was set at 3 days by DOE based on the time typically required to drill through the Castile and cement intermediate casing (see WPO #40520 p. 189). The Agency questioned the value of this parameter on the same basis as for the maximum period of uncontrolled flow. Lower periods of uncontrolled flow were documented in DOE's database and this parameter was potentially important in determining the magnitude of a direct brine release. This parameter was therefore included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the minimum period of uncontrolled borehole flow was evaluated in the Agency's SA by determining the change in the performance measure for high and low values of this parameter. The low value selected by the Agency was 1 day and the high value was 5 days, based on a DOE survey of current drilling practices (see WPO #43672 p. 9 and SA Report 1997 Appendix PD Section PD-2.4). The results indicated no sensitivity to changes in this parameter and this parameter was therefore identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.23 3433 PHUMOX3 - PHUMSIM: Humic Colloid Proportionality Constant in Salado Brine

This parameter is the proportionality constant for sorption of +3 actinides to humic colloids in Salado brine. It was defined, determined, and used by DOE in the same way as parameter PHUMOX3 - PHUMCIM for Castile brine discussed in Section 5.20 above; however, parameter

PHUMOX3 - PHUMSIM was treated as a constant in the CCA with a value of 0.19 rather than as a sampled variable. The Agency considered this parameter to be potentially important in computing brine releases and included it in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in this humic colloid proportionality constant was studied by the Agency in the same two sensitivity analyses described in Section 5.20 and in the SA Report (1997). The results indicated that the PA results are not sensitive to changes in the humic colloid proportionality constants. Because of a low sensitivity, this parameter was identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.24 3470 BLOWOUT - GAS_MIN: DBR Cutoff Gas Flow Rate

Direct brine releases are assumed by DOE to occur over a minimum of 3 days and then cease when either the gas flow rate drops below the value prescribed by this cutoff gas flow rate parameter, or when flow occurs in excess of 11 days, whichever occurs first. The cutoff gas flow rate was treated by DOE as a constant with a value of 100 mscf/day (100,000 standard cubic feet per day), which DOE considered to be a rate that a driller could readily control (see WPO #40520 p. 189). The Agency questioned the value of this parameter because of its lack of a documented source and because of its potential importance in determining the magnitude of a direct brine release. This parameter was therefore included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the cutoff gas flow rate was evaluated in the Agency's SA by determining the change in the performance measure for high and low values of this parameter. The low value selected by the Agency was 50 mscf/day and is equal to half of the CCA value. The high end was 200 mscf/day and is twice the CCA value (see SA Report 1997 Appendix PD Section PD-2.2). This range was considered by the Agency to provide an adequate test of sensitivity. The results showed no sensitivity to changes in the value of this parameter (see SA Report 1997 Table 3.2-1). This parameter was therefore identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.25 3317 PU - PROPMIC: Microbial Colloid Proportionality Constant for Plutonium

This parameter is the proportionality constant for sorption of plutonium ions to microbial colloids. It is defined as the ratio of the moles of plutonium sorbed on microbial colloids to the moles of plutonium remaining in solution. Plutonium and americium dominate the mobile radionuclide inventory and are the most important in evaluating releases. Values of this proportionality constant for americium are discussed in Section 5.33 below. Values for this proportionality constant were determined based on experiments conducted for the WIPP at Brookhaven National Laboratory. These values are assigned to actinides independent of oxidation state and brine type because, for living organisms, actinide uptake and toxicity are more closely associated with element type than with these variables. The parameter PU - PROPMIC was treated as a constant in the CCA with a value of 0.3, although a range of values for this parameter was identified in DOE's documentation (see WPO #35856 Table 1). The Agency considered this parameter to be potentially important in computing actinide solubility and questioned whether its uncertainty had been adequately captured in the CCA. This parameter was therefore included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the microbial colloid proportionality constants was studied by the Agency in two sensitivity analyses. In the first of these analyses, the values of this constant were simultaneously changed along with the values of other parameters associated with actinide solubility (see SA Report 1997 Appendix PD Section PD-4.1). In the second analysis, the values of this constant were varied alone (see SA Report 1997 Appendix PD Section PD-4.3). In both analyses the proportionality constants for both plutonium and americium were simultaneously assigned high or low values equal to the extremes of the ranges identified in the aforementioned DOE documentation. The results of these analyses are summarized in the SA Report (1997 Table 3.4-1). Although an average 51% change in the performance measures was found in the first analysis when other parameters were also changed, only a 4% change was found in the second analysis when only the microbial colloid proportionality constants were changed. This indicates that the microbial colloid proportionality constants were not the primary source of the 51% change in the first analysis, and that the PA results are not sensitive to changes in these parameters. Because of a low sensitivity, this parameter was therefore identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.26 3405 SOLMOD6 - SOLCIM: U (VI) Solubility in Castile Brine

This parameter is the expected solubility of uranium in the +6 oxidation state in Castile brine. The same constant value of 8.8 E-6 moles/liter, based on literature reviews, was used by DOE in the CCA for both Castile and Salado brines. The Agency considered this parameter to be potentially important in computing the uranium content of brine releases and questioned whether its value was applicable to WIPP brines. This parameter was therefore included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the sampled solubility calculated in the PA model to changes in the principal input parameters was studied by the Agency by simultaneously varying the values of those parameters for all actinides, oxidation states, and brines (see SA Report 1997 Appendix PD Section PD-4.1). For uranium +6 these were the SOLU6 - SOLSIM and SOLU6 - SOLCIM parameters (defined below), the microbial colloid proportionality constants (PROPMIC; see Sections 5.25 and 5.33), and the humic colloid proportionality constants (PHUMSIM and PHUMCIM; see Sections 5.20 and 5.23). SOLU6 - SOLSIM and SOLU6 - SOLCIM are defined in the following equations:

For uranium +6 in Salado brine:

$$\text{Sampled Solubility used in CCA} = \text{SOLMOD6-SOLSIM} \times 10^{\text{SOLU6-SOLSIM}}$$

For uranium +6 in Castile brine:

$$\text{Sampled Solubility used in CCA} = \text{SOLMOD6-SOLCIM} \times 10^{\text{SOLU6-SOLCIM}}$$

SOLU6 - SOLSIM and SOLU6 - SOLCIM are therefore high and low values used as powers of ten to define the range over which uranium +6 solubility was sampled by DOE for the CCA. The parameters SOLMOD6 - SOLSIM and SOLMOD6 - SOLCIM are the expected uranium +6 solubility values for Salado and Castile brines, respectively. As shown in the equations, solubility values are sampled by combining parameters for both range of solubility and expected solubility value, rather than by sampling directly from a single parameter. The same range of values was used by DOE for both SOLU6 - SOLSIM and SOLU6 - SOLCIM as well as for all other actinides, oxidation states, and brines, reflecting a lack of detailed knowledge of these parameters.

Because of the potential importance of parameter SOLMOD6 - SOLCIM in calculating direct radionuclide releases and the Agency's questions regarding the technical approach taken by DOE to determine the expected solubility of uranium +6 in Castile brine, a mandated constant value of 4.6 E-3 moles/liter was identified for this parameter in the Agency's letter of April 25, 1997 for use in the PAVT (Trovato 1997C Enclosure 2). The Agency did not provide a range of values for this parameter because sampling of uranium +6 solubilities is conducted by sampling another parameter, SOLU6 - SOLCIM, as described above. For similar reasons, the Agency also did not provide a range of values for the other SOLMOD parameters discussed below. The Agency's mandated value was calculated for Castile brine based on the solubility of the uranium mineral schoepite ($UO_3 \cdot 2H_2O$) using the USGS PHREEQC model and assuming chemical conditions based on equilibrium between brucite and hydromagnesite (EPA, 1998c, Docket No. A-93-02, V-B-17). This calculation provided a conservative estimate because the uranium +6 concentrations calculated for schoepite solubility are greater than the concentrations measured in DOE's brine experiments. These brine experiments were conducted under alkaline conditions expected to be representative of the repository environment. In view of the lack of other WIPP-specific values, the Agency considered this approach acceptable. The Agency did not mandate changes in SOLU6 - SOLCIM for the PAVT because the range of values for that sampled parameter was considered sufficiently broad to capture the uncertainty in parameter SOLMOD6 - SOLCIM.

Subsequent to the Agency's aforementioned April 25, 1997 letter, additional experimental results provided by DOE indicated that uranium +6 solubilities in high ionic strength WIPP brines were lower than the value of 8.8 E-6 moles/liter used in the CCA (see Kruger 1997; WPO # 44625; WPO # 45115). Based on this new information as well as the original basis used by DOE to establish the CCA parameter values (see WPO # 36488), the Agency informed DOE that the uranium +6 solubilities used in the CCA for Castile and Salado brines (parameters 3405 and 3409) were considered adequate and did not need to be changed in the PAVT.

5.27 3409 SOLMOD6 - SOLSIM: U(VI) Solubility in Salado Brine

This parameter is the expected solubility of uranium in the +6 oxidation state in Salado brine. The same constant value of 8.8 E-6 moles/liter, based on literature reviews, was used by DOE in the CCA for both Castile and Salado brines. The Agency considered this parameter as well as the parallel parameter for Castile brine (see Section 5.26) to be potentially important in computing the uranium content of brine releases and questioned whether the assigned value was applicable to WIPP brines. This parameter was therefore included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

Because of the potential importance of the parameter SOLMOD6 - SOLSIM in calculating direct radionuclide releases and the Agency's questions regarding the technical approach taken by DOE to determine the expected solubility of uranium +6 in Salado brine, a mandated value of 3.7 E-5 moles/liter was identified for this parameter in the Agency's letter of April 25, 1997 for use in the PAVT (Trovato 1997C Enclosure 2). The Agency's mandated value was calculated for Salado brine in the same manner as described for Castile brine in Section 5.26. This calculation provided a conservative estimate as mentioned above. However, as described in Section 5.26, subsequent to the Agency's aforementioned April 25, 1997 letter, additional experimental results provided by DOE allowed the Agency to conclude that the uranium +6 solubilities used in the CCA for Castile and Salado brines (parameters 3405 and 3409) were adequate and did not need to be changed in the PAVT.

5.28 3402 SOLMOD3 - SOLCIM: Oxidation State +III Solubility in Castile Brine (3406 SOLMOD3 - SOLSIM)

This parameter is used by DOE in the CCA as the expected solubility of all actinides in the +3 oxidation state in Castile brine. The solubility of americium +3 in Castile brine was used by DOE as a surrogate for the solubility of other +3 actinides because of their limited or inadequate data base. A constant value of 6.52 E-8 moles/liter, based on FMT computer code modeling, was used by DOE for this parameter. The Agency's analysis of the FMT code used to calculate solubilities revealed incorrect solubility estimates because the database used as an input to FMT was in error, as were the resulting CCA calculations (EPA 1998d, Appendix A). Because of these errors and because of the potential importance of this parameter in calculating the concentration of +3 actinides in brine releases, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

DOE assumed in the CCA that, under the expected reducing repository conditions, plutonium dissolved in the Castile and Salado brines would exist predominantly in either the +3 or +4 oxidation states and assigned equal probabilities to each of these states in the PA. The repository inventory includes large quantities of reducing agents in the form of metallic iron, organic matter, and organic chemicals. These reductants are expected to rapidly consume any available oxygen present in the repository atmosphere shortly after closure, producing reducing conditions. Under reducing conditions, plutonium is expected to be stable in either the +3 or +4 oxidation states based on chemical equilibrium arguments. In confirmation of this expectation, experimental studies conducted by DOE have shown that Pu +6 is rapidly reduced to lower oxidation states by direct reactions with iron and organic compounds (WPO # 35197). Also, stabilization of plutonium in the +6 oxidation state by carbonate is not expected to occur in the repository because reactions with the magnesium oxide backfill should limit CO_2 (g) to very low partial pressures based on chemical equilibrium calculations.

Experimental studies indicate that both Pu +3 and Pu +4 are produced by the reduction of Pu +6 with various metallic iron and organic compounds. However, the predominant oxidation state expected for the repository conditions cannot be defined with absolute certainty based on the experimental studies or equilibrium model calculations. Consequently, DOE assumed that both Pu +3 and Pu +4 were possible and included both in the PA calculations.

Upon review, the Agency concurs with DOE's conclusions regarding plutonium oxidation states and believes that the foregoing approach is reasonable and consistent with current knowledge of plutonium redox chemistry and expected repository conditions.

A mandated value of 1.38 E-8 moles/liter was identified for parameter SOLMOD3 - SOLCIM in the Agency's letter of April 25, 1997 for use in the PAVT (Trovato 1997C Enclosure 2). This mandated value was calculated for Castile brine using the corrected database to execute the FMT model and assuming chemical conditions based on equilibrium between brucite and hydromagnesite rather than between brucite and magnesite (EPA 1998d, Appendix A, Table 4). This calculation is based on the Pitzer activity coefficient formalism and is considered appropriate for high ionic strength solutions. As a result of the model corrections, the calculated solubility was lower than that used by DOE in the CCA. This change will result in smaller concentrations of actinides in solution and decreased actinide releases.

Parameter 3406 SOLMOD3 - SOLSIM is the expected solubility of all actinides in the +3 oxidation state in Salado brine. Although it was inadvertently not included in the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A), DOE was required by the Agency's letter of April 25, 1997 to use an alternate value for this parameter in the PAVT (Trovato 1997C Enclosure 2). The solubility of americium +3 in Salado brine was used by DOE as a surrogate for the solubility of other +3 actinides because of their limited or inadequate data base. A constant value of 5.82 E-8 moles/liter, based on FMT modeling, was used by DOE for this parameter. The Agency's concerns for this parameter stem from the aforementioned database errors used to execute the FMT model (EPA 1998d, Appendix A) and the potential importance of this parameter in calculating the actinide content of brine releases. A mandated value of 1.2 E-7 moles/liter was identified for parameter SOLMOD3 - SOLSIM in the Agency's letter of April 25, 1997 for use in the PAVT (Trovato 1997C Enclosure 2). The Agency's mandated value was calculated for Salado brine using the corrected database used to execute the FMT model and assuming chemical conditions based on equilibrium between brucite and hydromagnesite (EPA 1998d, Appendix A, Table 3). This calculation is based on the Pitzer activity coefficient formalism and is considered appropriate for high ionic strength solutions. As a result of the model corrections, the calculated solubility was higher than that used by DOE in the CCA. This change will result in greater concentrations of actinides in solution and increased actinide releases. Ranges for the two SOLMOD3 parameters were not specified by the Agency because solubility is sampled in the CCA using other parameters, as explained in Section 5.26.

5.29 3403 SOLMOD4 - SOLCIM: Oxidation State +IV Solubility in Castile Brine

This parameter is used by DOE in the CCA as the expected solubility of all actinides in the +4 oxidation state in Castile brine. The solubility of thorium +4 was used by DOE as a surrogate for the solubility of other +4 actinides because of their limited or inadequate data base. A constant value of 6.00 E-9 moles/liter, based on FMT modeling, was used by DOE for this parameter. As mentioned in Section 5.28, the Agency's analysis of the FMT computer code used to calculate solubilities revealed incorrect solubility estimates because the database used for as an input to FMT was in error, as were the resulting CCA calculations (EPA 1998d, Appendix A). Because of these errors and because of the potential importance of this parameter in calculating the concentration of +4 actinides in brine releases, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

A mandated value of 4.1 E-8 moles/liter was identified for parameter SOLMOD4 - SOLCIM in the Agency's letter of April 25, 1997 for use in the PAVT (Trovato 1997C Enclosure 2). The Agency's mandated value was calculated for Castile brine using the corrected FMT database values and assuming chemical conditions based on equilibrium between brucite and hydromagnesite (EPA 1998d, Appendix A, Table 4). This calculation is based on the Pitzer activity coefficient formalism and is considered appropriate for high ionic strength solutions. As a result of the model corrections, the calculated solubility was higher than that used by DOE in the CCA. This change will result in greater concentrations of actinides in solution and increased actinide releases. A range for this SOLMOD4 parameter was not specified by the Agency because solubility is sampled in the CCA using other parameters, as explained in Section 5.26.

5.30 3407 SOLMOD4 - SOLSIM: Oxidation State +IV Solubility in Salado Brine

This parameter is used by DOE in the CCA as the expected solubility of all actinides in the +4 oxidation state in Salado brine. The solubility of thorium +4 was used by DOE as a surrogate for the solubility of other +4 actinides because of their limited or inadequate data base. A constant value of 4.4 E-6 moles/liter, based on FMT modeling, was used by DOE for this parameter. As mentioned in Section 5.28, the Agency's analysis of the FMT code as used to calculate solubilities revealed incorrect solubility estimates because the database used for as an input to FMT was in error, as were the resulting CCA calculations (EPA 1998d, Appendix A). Because of these errors and because of the potential importance of this parameter in calculating the concentration of +4 actinides in brine releases, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

Because of the potential importance of this parameter in calculating radionuclide releases and to provide an opportunity to use the corrected database used to execute the FMT model in performance assessment, a mandated value of 1.3 E-8 moles/liter was identified for parameter SOLMOD4 - SOLSIM in the Agency's letter of April 25, 1997 for use in the PAVT (Trovato 1997C Enclosure 2). The Agency's mandated value was calculated for Salado brine using the corrected FMT model and assuming chemical conditions based on equilibrium between brucite and hydromagnesite (EPA 1998d, Appendix A, Table 3). This calculation is based on the Pitzer activity coefficient formalism and is considered appropriate for high ionic strength solutions. As a result of the model corrections, the calculated solubility was lower than that used by DOE in the CCA. This change will result in smaller concentrations of actinides in solution and decreased actinide releases. A range for this SOLMOD4 parameter was not specified by the Agency because solubility is sampled in the CCA using other parameters, as explained in Section 5.26.

5.31 3404 SOLMOD5 - SOLCIM: Oxidation State +V Solubility in Castile Brine

This parameter is used by DOE in the CCA as the expected solubility of all actinides in the +5 oxidation state in Castile brine. The solubility of neptunium +5 was used by DOE as a surrogate for the solubility of other +5 actinides because of their limited or inadequate data base. A constant value of 2.2 E-6 moles/liter, based on FMT modeling, was used by DOE for this parameter. As mentioned in Section 5.28, the Agency's analysis of the FMT code used to calculate solubilities revealed incorrect solubility estimates because the database used as an input to FMT was in error, as were the resulting CCA calculations (EPA 1998d, Appendix A). Because of these errors and because of the potential importance of this parameter in calculating the concentration of +5 actinides in brine releases, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

A mandated value of 4.8 E-7 moles/liter was identified for parameter SOLMOD5 - SOLCIM in the Agency's letter of April 25, 1997 for use in the PAVT (Trovato 1997C Enclosure 2). The Agency's mandated value was calculated for Castile brine using the corrected FMT model and assuming chemical conditions based on equilibrium between brucite and hydromagnesite (EPA 1998d, Appendix A, Table 4). This calculation is based on the Pitzer activity coefficient formalism and is considered appropriate for high ionic strength solutions. As a result of the model corrections, the calculated solubility was lower than that used by DOE in the CCA. This change will result in smaller concentrations of actinides in solution and decreased actinide releases. A range for this SOLMOD5 parameter was not specified by the Agency because solubility is sampled in the CCA using other parameters, as explained in Section 5.26.

5.32 3408 SOLMOD5 - SOLSIM: Oxidation State +V Solubility in Salado Brine

This parameter is used by DOE in the CCA as the expected solubility of all actinides in the +5 oxidation state in Salado brine. The solubility of neptunium +5 was used by DOE as a surrogate for the solubility of other +5 actinides because of their limited or inadequate data base. A constant value of 2.3 E-6 moles/liter, based on FMT modeling, was used by DOE for this parameter. As mentioned in Section 5.28, the Agency's analysis of the FMT code to calculate solubilities revealed incorrect solubility estimates because the database used for as an input to FMT was in error, as were the resulting CCA calculations (EPA 1998d, Appendix A). Because of these errors and because of the potential importance of this parameter in calculating the concentration of +5 actinides in brine releases, it was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

A mandated value of 2.4 E-7 moles/liter was identified for parameter SOLMOD4 - SOLSIM in the Agency's letter of April 25, 1997 for use in the PAVT (Trovato 1997C Enclosure 2). The Agency's mandated value was calculated for Salado brine using the corrected FMT model and assuming chemical conditions based on equilibrium between brucite and hydromagnesite (EPA 1998d, Appendix A, Table 3). This calculation is based on the Pitzer activity coefficient formalism and is considered appropriate for high ionic strength solutions. As a result of the model corrections, the calculated solubility was lower than that used by DOE in the CCA. This change will result in smaller concentrations of actinides in solution and decreased actinide releases. A range for this SOLMOD5 parameter was not specified by the Agency because solubility is sampled in the CCA using other parameters, as explained in Section 5.26.

5.33 3311 AM - PROPMIC: Microbial Colloid Proportionality Constant for Americium

This parameter is the proportionality constant for sorption of americium ions to microbial colloids. It is defined as the ratio of the moles of americium sorbed on microbial colloids to the moles of americium remaining in solution. This parameter is treated in the same manner as parameter PU - PROPMIC described in Section 5.25 above. Plutonium and americium dominate the mobile radionuclide inventory and are the most important in evaluating releases. The parameter AM - PROPMIC was treated as a constant in the CCA with a value of 3.6, although a range of values for this parameter was identified in DOE's documentation (see WPO #35856 Table 1). The Agency considered this parameter to be potentially important in computing actinide solubility and questioned whether its uncertainty had been adequately captured in the CCA. This parameter was then included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the microbial colloid proportionality constants was studied by the Agency in two sensitivity analyses described in Section 5.25. In both analyses the proportionality constants for both plutonium and americium were simultaneously assigned high or low values corresponding to the extremes of the ranges identified in the aforementioned DOE documentation. The results of these analyses are summarized in the SA Report (1997 Table 3.4-1). Although an average 51% change in the performance measures was found in the first analysis when other parameters were also changed, only a 4% change was found in the second analysis when only the microbial colloid proportionality constants were changed. This indicates that the microbial colloid proportionality constants were not the primary source of the 51% change in the first analysis, and that the PA results are not sensitive to changes in these parameters. Because of a low sensitivity, this parameter was therefore identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.34 3482 AM+3 - MKD_AM: Matrix Partition Coefficient for Americium +III

This parameter is the solid-liquid partition coefficient (K_d) for americium +3 in the Culebra dolomite. DOE developed values for this parameter based on laboratory experiments performed at Los Alamos National Laboratory and Sandia National Laboratories (see WPO #38801). This parameter was treated as a sampled variable in the CCA with a uniform distribution and a range of 0.02 m^3/kg to 0.5 m^3/kg. Because of the potential importance of this and other K_d values in predicting the migration of actinides in the Culebra dolomite to the accessible environment, a detailed evaluation of DOE's methodology for determining K_d values was conducted by the Agency (EPA, 1997b). Concerns identified in the Agency's evaluation, discussed below, caused the Agency to question DOE's technical approach, and because of the importance of americium in WIPP's actinide inventory, included the K_d for americium +3 in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

In the aforementioned Agency evaluation (EPA, 1997b), the actinide K_ds used by DOE in the CCA were compared with literature values, DOE's experimental approach was critically reviewed, and DOE's experiments on the effects of organic ligands were reviewed. The literature review indicated that in most cases the actinide K_ds determined for the WIPP brines fell into the lower end of the range of values reported for sands, loams, and clayey soils. However, less retention of the actinides on solids in a high ionic strength brine would be expected than in more dilute solutions because of swamping of available adsorption sites by the high concentrations of the ionic species present in the brine, and also because of the lower sorptive capacity of the dolomitic rock (see EPA, 1997b). Lower K_d values are more conservative because higher actinide concentrations are predicted to remain in solution and remain available for transport.

In reviewing DOE's experimental work on K_ds, the Agency concluded that the experimental procedure, including the use of crushed Norwegian dolomite as well as crushed Culebra dolomite, was adequate. Crushed samples are often used in K_d experiments to minimize imprecision resulting from variabilities in surface chemical properties, and given the long time period over which actinide migration occurs in the Culebra, DOE's assertion that fluid moving through this dolomite will eventually be exposed to the same surface to volume ratio that was used in the experiments is not unreasonable. Also, the Agency agrees with DOE's objective of using the purer Norwegian dolomite to provide more conservative measures of K_ds by focusing on the mineral dolomite and reducing the effects of impurities such as clays in the Culebra dolomite that could tend to increase the measured values.

However, the Agency identified a lack of documentation that equilibrium had been reached in the experiments and that the effects of actinide concentrations on the measured K_ds were considered (see EPA, 1997b). Although this lack of documentation was of concern, it was not considered a major technical issue. The DOE's experiments were continued for 8 weeks rather than the 48 hours or less normally used for equilibration in K_d experiments, and are considered by the Agency to have an adequate duration. Also, the low actinide concentrations used in the experiments essentially precluded the formation of precipitates and the loss of actinides from solution by that mechanism.

The Agency also noted that the effects of the MgO backfill and the more alkaline brine solution it would create were not considered in the experiments. Although there is some uncertainty about the effects of a more alkaline solution on adsorption to dolomite, for which less information is available than for other geologic media, the adsorption of cationic species generally increases with increasing pH. Calcite, which is chemically similar to dolomite and may be considered an analog for that mineral, does exhibit this tendency for increasing adsorption with increasing pH (see EPA, 1997b). The use of a lower pH brine in the K_d experiments than would actually be present in the repository is therefore expected to underestimate K_d values and provide more conservative calculations of potential releases by increasing the radionuclide fraction remaining dissolved in the brine.

The uncertainty of DOE's experimental results was increased when the K_d experiments for americium +3 failed (for the reasons described in WPO # 38801), and K_ds measured for plutonium +5 were used to represent americium +3. Also, because americium +3 was to be the analog for plutonium +3, the K_ds measured for plutonium +5 were also used for plutonium +3. Although the Agency would prefer to not use surrogates for these parameters, particularly surrogates with different oxidation states, the uncertainty in these parameters has been adequately captured within the aforementioned range of 0.02 to 0.5 m^3/kg sampled in PA.
The Agency's review of DOE's experimental work on organic ligands indicated that although at low ligand concentrations some actinide K_ds increased relative to values determined in the absence of organics, at higher ligand concentrations actinide K_ds generally showed decreased values. The results of the ligand experiments were not used by DOE in deriving the K_d ranges used in the CCA based on the hypothesis that a surplus of metallic cations in the repository brine will form complexes with the ligands, making them generally unavailable for affecting actinide speciation. DOE tested the validity of this hypothesis by using the FMT model to perform speciation calculations comparing the effects of organic ligands in the experimental solutions with those expected under repository conditions (Novak et al. 1996). Results from the FMT calculations were found to be generally consistent with the aforementioned hypothesis.

Although the Agency recognizes that the FMT calculations are not completely descriptive of the expected repository conditions, consideration of K_ds reported in the literature, the expected increased adsorption under alkaline conditions resulting from MgO backfill reactions, and the results of the speciation calculations support use of the K_d ranges used by DOE in the CCA (see EPA, 1997b). However, the K_d values obtained by DOE appear to be logarithmically distributed, and the Agency questions DOE's use of a uniform distribution for K_ds in the CCA (EPA, 1997b). Because of the Agency's question regarding the form of the distribution, and because the actinide K_ds range over more than an order of magnitude, DOE was required by the Agency's letter of April 25, 1997 (Trovato 1997C Enclosure 2) to treat this parameter as a sampled value in the PAVT with a loguniform rather than a uniform distribution, while maintaining the same range of values as used in the CCA. Use of a loguniform distribution provides equal weight in sampling across the range of values and conservatively reduces the median value of this parameter, thereby increasing the average mass of actinides in solution.

5.35 3480 PU+3 - MKD_PU: Matrix Partition Coefficient for Plutonium +III

This parameter is the solid-liquid partition coefficient (K_d) for plutonium +3 in the Culebra dolomite. DOE developed values for this parameter based on laboratory experiments using plutonium +5 as an analog (see WPO #38801). This parameter was treated as a sampled variable in the CCA with a uniform distribution and a range of 0.02 m^3/kg to 0.5 m^3/kg. This is the same range as for americium +3, for which plutonium +5 was also an analog. A detailed discussion of the Agency's review and conclusions regarding DOE's K_d values is presented in Section 5.34 above. Because of the potential importance of this and other K_d values in predicting the migration of actinides in the Culebra dolomite to the accessible environment, and because of concerns identified in the Agency's evaluation of the technical basis for this parameter, the K_d for plutonium +3 was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

An overview of the Agency's technical evaluation of DOE's K_d values is presented in Section 5.34. As a result of this evaluation, the Agency concluded that the ranges of K_d values used in the CCA were appropriate and adequately reflected the uncertainty in this parameter. However, the Agency questioned DOE's use of a uniform distribution for K_ds in the CCA. Previous reviews of K_ds reported in the literature have found this parameter to be logarithmically distributed (see EPA, 1997b), and because the actinide K_ds range over more than an order of magnitude, DOE was required by the Agency's letter of April 25, 1997 (Trovato 1997C Enclosure 2) to treat this parameter as a sampled value in the PAVT with a loguniform rather than a uniform distribution, while maintaining the same range of values as used in the CCA. Use of a loguniform distribution provides equal weight in sampling across the range of values and conservatively reduces the median value of this parameter, thereby increasing the average mass of actinides in solution.

5.36 3481 PU+4 - MKD_PU: Matrix Partition Coefficient for Plutonium +IV

This parameter is the solid-liquid partition coefficient (K_d) for plutonium +4 in the Culebra dolomite. DOE developed values for this parameter based on laboratory experiments using thorium +4 as an analog (see WPO #38801). This parameter was treated as a sampled variable in the CCA with a uniform distribution and a range of 0.9 m^3/kg to 20 m^3/kg. This is the same range as for uranium +4, for which thorium +4 (Parameter 3478 TH+4 - MKD_TH) was also an analog. A detailed discussion of the Agency's review and conclusions regarding DOE's K_d values is presented in Section 5.34 above. Because of the potential importance of this and other K_d values in predicting the migration of actinides in the Culebra dolomite to the accessible environment, and because of concerns identified in the Agency's evaluation of the technical basis for this parameter, the K_d for plutonium +4 was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

An overview of the Agency's technical evaluation of DOE's K_d values is presented in Section 5.34. As a result of this evaluation, the Agency concluded that the ranges of K_d values used in the CCA were appropriate and adequately reflected the uncertainty in this parameter. However, the Agency questioned DOE's use of a uniform distribution for K_ds in the CCA. Previous reviews of K_ds reported in the literature have found this parameter to be logarithmically distributed (see EPA, 1997b), and because the actinide K_ds range over more than an order of magnitude, DOE was required by the Agency's letter of April 25, 1997 (Trovato 1997C Enclosure 2) to treat this parameter as a sampled value in the PAVT with a loguniform rather than a uniform distribution, while maintaining the same range of values as used in the CCA. Use of a loguniform distribution provides equal weight in sampling across the range of values and conservatively reduces the median value of this parameter, thereby increasing the average mass of actinides in solution.

5.37 3479 U+4 - MKD_U: Matrix Partition Coefficient for Uranium +IV

This parameter is the solid-liquid partition coefficient (K_d) for uranium +4 in the Culebra dolomite. DOE developed values for this parameter based on laboratory experiments using thorium +4 as an analog (see WPO #38801). This parameter was treated as a sampled variable in the CCA with a uniform distribution and a range of 0.9 m^3/kg to 20 m^3/kg. This is the same range as for plutonium +4, for which thorium +4 was also an analog. A detailed discussion of the Agency's review and conclusions regarding DOE's K_d values is presented in Section 5.34 above. Because of the potential importance of this and other K_d values in predicting the migration of actinides in the Culebra dolomite to the accessible environment, and because of concerns identified in the Agency's evaluation of the technical basis for this parameter, the K_d for uranium +4 was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

An overview of the Agency's technical evaluation of DOE's K_d values is presented in Section 5.34. As a result of this evaluation, the Agency concluded that the ranges of K_d values used in the CCA were appropriate and adequately reflected the uncertainty in this parameter. However, the Agency questioned DOE's use of a uniform distribution for K_ds in the CCA. Previous reviews of K_ds reported in the literature have found this parameter to be logarithmically distributed (see EPA, 1997b), and because the actinide K_ds range over more than an order of magnitude, DOE was required by the Agency's letter of April 25, 1997 (Trovato 1997C Enclosure 2) to treat this parameter as a sampled value in the PAVT with a loguniform rather than a uniform distribution, while maintaining the same range of values as used in the CCA. Use of a loguniform distribution provides equal weight in sampling across the range of values and conservatively reduces the median value of this parameter, thereby increasing the average mass of actinides in solution.

5.38 3475 U+6 - MKD_U: Matrix Partition Coefficient for Uranium +VI

This parameter is the solid-liquid partition coefficient (K_d) for uranium +6 in the Culebra dolomite. DOE developed values for this parameter based on laboratory experiments (see WPO #38801). This parameter was treated as a sampled variable in the CCA with a uniform distribution and a range of 0.00003 m^3/kg to 0.03 m^3/kg. A detailed discussion of the Agency's review and conclusions regarding DOE's K_d values is presented in Section 5.34. Because of the potential importance of this and other K_d values in predicting the migration of actinides in the Culebra dolomite to the accessible environment, and because of concerns identified in the Agency's evaluation of the technical basis for this parameter, the K_d for uranium +6 was included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

An overview of the Agency's technical evaluation of DOE's K_d values is presented in Section 5.34. As a result of this evaluation, the Agency concluded that the ranges of K_d values used in the CCA were appropriate and adequately reflected the uncertainty in this parameter. However, the Agency questioned DOE's use of a uniform distribution for K_ds in the CCA. Previous reviews of K_ds reported in the literature have found this parameter to be logarithmically distributed (see EPA, 1997b), and because the actinide K_ds range over more than an order of magnitude, DOE was required by the Agency's letter of April 17, 1997 (Trovato 1997B Enclosure 2) to treat this parameter as a sampled value in the PAVT with a loguniform rather than a uniform distribution, while maintaining the same range of values as used in the CCA. Use of a loguniform distribution provides equal weight in sampling across the range of values and conservatively reduces the median value of this parameter, thereby increasing the average mass of actinides in solution.

5.39 656 WAS_AREA - GRATMICH: Gas Generation Rate due to Microbial Action under Humid Conditions

The gas generation due to microbial action under humid (brine unsaturated) conditions was estimated by DOE based on laboratory studies of microbial consumption of cellulosics at Brookhaven National Laboratory (see CCA Docket: A-93-02, II-G-1, Volume X, Appendix MASS p. MASS-55). DOE treated this parameter as a sampled variable in the CCA with a uniform distribution and a range of zero to 1.268 E-9 moles/kg-s (see WPO #34923 p. 1). Because of the potential importance of this parameter in calculating repository gas pressures, the Agency questioned whether its uncertainty had been adequately captured in the CCA. This parameter was therefore included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the gas generation due to microbial action under humid conditions was studied by the Agency in a sensitivity analysis (see SA Report 1997 Appendix PD Section PD-1.22). In this analysis the value of this parameter was set equal to the extreme values of the range sampled by DOE in the CCA. No sensitivity of the performance measures to changes in this parameter were found (see SA Report 1997 Table 3.1-1). Because of a lack of sensitivity, this parameter was identified in the Agency's letter of April 25, 1997 as being no longer in question (Trovato 1997C Enclosure 1).

5.40 657 WAS_AREA - GRATMICI: Gas Generation Rate due to Microbial Action under Inundated Conditions

The gas generation due to microbial action under inundated (brine saturated) conditions was estimated by DOE based on laboratory studies of microbial consumption of cellulosics at Brookhaven National Laboratory (see CCA Docket: A-93-02, II-G-1, Volume X, Appendix MASS p. MASS-55). DOE treated this parameter as a sampled variable in the CCA with a uniform distribution and a range of 3.17 E-10 mole/kg-s to 9.51 E-9 moles/kg-s (see CCA Docket: A-93-02, II-G-1, Volume XI, Appendix PAR p. PAR-21 and WPO #34928 p. 1). Because of the potential importance of this parameter in calculating repository gas pressures, the Agency questioned whether its uncertainty had been adequately captured in the CCA. This parameter was therefore included in Enclosure 4 of the Agency's March 19, 1997 letter as requiring further evaluation (Trovato 1997A).

The sensitivity of the PA model to changes in the gas generation due to microbial action under inundated conditions was studied by the Agency in a sensitivity analysis (see SA Report 1997 Appendix PD Section PD-1.23). In this analysis the value of this parameter was set equal to the extreme values of the range sampled by DOE in the CCA. The average change in the performance measures resulting from changes in the value of this parameter was found to be 1% and was not considered significant by the Agency (see SA Report 1997 Table 3.1-1). Because of this low sensitivity, this parameter was identified in the Agency's letter of April 17, 1997 as being no longer in question (Trovato 1997B Enclosure 1).

6.0 SUMMARY AND CONCLUSIONS

This report describes the disposition of 58 parameters used by DOE in the CCA PA that were found to be inadequately supported following an extensive review of DOE's parameter database by the Agency. These parameters were identified to DOE in Enclosures 2, 3, and 4 of the Agency's letter of March 19, 1997 and are discussed in Sections 3, 4, and 5, respectively, of this report (Trovato 1997A). These parameters were identified because they were potentially important to the results of the PA and because they lacked supporting data, they had different values or ranges than were supported in the DOE database, or they had questionable values or ranges.

Each of these parameters was further reviewed by the Agency and dispositioned either by being resolved and no longer in question, or by being included in the mandated PAVT with revised values, ranges, or distributions determined by the Agency. The parameters and their dispositions are discussed in Sections 3, 4, and 5 of this report and summarized in Tables 6.1 through 6.3. Some parameters were found to be no longer in question because they were either found to be not sensitive in the Agency's sensitivity analysis, or because they were accepted after review of additional documentation provided by DOE or through the Agency's studies. Other parameters were no longer in question because they were eliminated from the PA model in response to an Agency-mandated change, or they were found to not have been used in the CCA version of the PA model. In the last case, if the parameter was considered important, alternate parameters were identified and changed in the PAVT to achieve the Agency's objective in questioning the original parameter.

After making the necessary adjustments to allow for model changes, a final list of 22 parameters that were to be changed in the PAVT was developed and is presented in Table 6.4. This table also summarizes the parameter values, ranges, and distributions used in the PAVT as well as the original values used in the CCA. The basis for selecting each parameter, value, range, and distribution is presented in Sections 3, 4, and 5 of this report.

Table 6.1. Parameters Lacking Supporting Data

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
1	3245	BLOWOUT-CEMENT	Waste cementation strength	Change required for PAVT in 4/25 letter but removed	Sensitive but removed due to change in model
2	3246	BLOWOUT-PARTDIA	Waste particle diameter	Required revision using expert elicitation process	Not appropriately justified
3	198	DRZ_1-PRMX_LOG	Intrinsic permeability in X-direction in disturbed rock zone	Change required for PAVT in 4/17 letter	Sensitive and not appropriately justified
4	2177	S_MB_139-DPHIMAX	Incremental increase in anhydrite porosity in Marker Bed 139	Removed in 4/25 letter	Documentation provided and accepted after review
5	2180	S_MB_139-PF_DELTA	Incremental pressure for full fracture development	Removed in 4/25 letter	Documentation provided and accepted after review
6	586	S_MB_139-PI_DELTA	Fracture initiation pressure increment	Removed in 4/25 letter	Documentation provided and accepted after review
7	2178	S_MB_139-KMAXLOG	Maximum permeability in altered anhydrite	Removed in 4/25 letter	Documentation provided and accepted after review
8	3134	BH_OPEN-PRMX_LOG	Intrinsic permeability in X-direction in open borehole	Removed in 4/25 letter	Not sensitive
9	2158	S_ANH_AB-DPHIMAX	Incremental increase in anhydrite porosity in beds A and B	Removed in 4/25 letter	Documentation provided and accepted after review
10	214	EXP_AREA-PRMX_LOG	Intrinsic permeability in X-direction in experimental area	Removed in 4/25 letter	Not sensitive
11	3473	BLOWOUT-THCK_CAS	Thickness of Castile brine pocket for direct brine release	Removed in 4/25 letter	Not sensitive
12	3456	BLOWOUT-RE_CAST	Radius of Castile brine pocket for direct brine release	Removed in 4/25 letter	Not sensitive
13	3194	CASTILER-GRIDFLO	Index for selecting brine pocket volume	Removed in 4/25 letter	Not used in CCA PA model - volume changed using other parameters

Table 6.2. Parameters with Different Values or Ranges

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
1	3493	GLOBAL-PBRINE	Probability of encountering pressurized brine	Change required for PAVT in 4/25 letter	Not appropriately justified
2	2254	BOREHOLE-TAUFAIL	Waste shear resistance	Change required for PAVT in 4/25 letter and 6/6 note to docket	Sensitive and not appropriately justified
3	3184	BH_SAND-PRMX_LOG	Long term intrinsic borehole permeability in X-direction	Change required for PAVT in 4/17 letter	Sensitive and not appropriately justified
4	2918	CASTILER-VOLUME	Castile brine pocket volume	Removed in 4/25 letter	Not used in CCA PA model - volume changed using compressibility and porosity adjustment
5	61	CASTILER-COMP_RCK	Castile brine pocket rock compressibility	Change required for PAVT in 4/17 letter	Not appropriately justified; used to change brine pocket volume

Table 6.3. Parameters with Questionable Values or Ranges

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
1	27	BOREHOLE-DOMEGA	Drill string angular velocity	Change required for PAVT in 4/25 letter	Sensitive and not appropriately justified
2	64	CASTILER-POROSITY	Castile brine pocket porosity	Removed in 4/25 letter	Not sensitive
3	66	CASTILER-PRESSURE	Castile brine pocket pore pressure	Removed in 4/25 letter	Not sensitive
4	259	PAN_SEAL-PRMX_LOG	Intrinsic permeability of panel seal in X-direction	Removed in 4/17 letter	Not sensitive
5	528	S_ANH_AB-POROSITY	Porosity of anhydrite beds A and B	Removed in 4/17 letter	Not sensitive
6	567	S_MB138-POROSITY	Porosity of anhydrite Marker Bed 138	Removed in 4/17 letter	Not sensitive
7	588	S_MB139-POROSITY	Porosity of anhydrite Marker Bed 139	Removed in 4/17 letter	Not sensitive
8	651	WAS_AREA-ABSROUGH	Waste area absolute roughness	Removed in 4/17 letter	Not sensitive and acceptable after review of documentation
9	653	WAS_AREA-COMP_RCK	Waste area rock compressibility	Removed in 4/17 letter	Not sensitive
10	1992	WAS_AREA-DIRNCCHW	Bulk density of iron containers in CH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review
11	1993	WAS_AREA-DIRNCRHW	Bulk density of iron containers in RH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review
12	2040	WAS_AREA-DIRNCHW	Average density of iron-based material in CH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review
13	2041	WAS_AREA-DCELLCHW	Average density of cellulosics in CH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
14	2274	WAS_AREA-DCELLRHW	Average density of cellulosics in RH waste	Removed in 4/17 letter	Sensitive, but documentation provided and accepted after review
15	2907	STEEL-CORRMCO2	Steel corrosion rate	Change required for PAVT in 4/17 letter	Not appropriately justified
16	3147	CONC_PLG-POROSITY	Borehole plug porosity	Removed in 4/17 letter	Not sensitive
17	3185	CONC_PLG-PRMX_LOG	Borehole plug permeability in X-direction	Change required for PAVT in 4/17 letter	Sensitive and not appropriately justified
18	3256	BLOWOUT-FGE	Gravity scaling factor	Change required for PAVT in 4/17 letter but removed	Removed due to change in model
19	3259	BLOWOUT-APORO	Waste permeability in CUTTINGS_S Model	Change required for PAVT in 4/25 letter but removed	Not used in CCA PA model -replaced with changes to parameters 663 WAS_AREA-PRMX_LOG and 2131 REPOSIT-PRMX_LOG
20	3429	PHUMOX3-PHUMCIM	Humic colloid proportionality constant	Removed in 4/25 letter	Not sensitive
21	3471	BLOWOUT-MAXFLOW	Maximum period of uncontrolled borehole flow	Removed in 4/25 letter	Sensitive, but documentation provided and accepted after review
22	3472	BLOWOUT-MINFLOW	Minimum period of uncontrolled borehole flow	Removed in 4/25 letter	Not sensitive
23	3433	PHUMOX3-PHUMSIM	Humic colloid proportionality constant	Removed in 4/25 letter	Not sensitive
24	3470	GLOWOUT-GAS_MIN	DBR cutoff gas flow rate	Removed in 4/25 letter	Not sensitive
25	3317	PU-PROPMIC	Microbial colloid proportionality constant for plutonium	Removed in 4/25 letter	Not sensitive
26	3405	SOLMOD6-SOLCIM	U(VI) solubility limit in Castile brine	Removed in 6/6 note to docket	Sensitive, but documentation provided and accepted after review

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
27	3409	SOLMOD6-SOLSIM	U(VI) solubility limit in Salado brine	Removed in 6/6 note to docket	Sensitive, but documentation provided and accepted after review
28a	3406	SOLMOD3-SOLCIM	Oxidation state +3 solubility limit in Castile brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
28b	3402	SOLMOD3-SOLSIM	Oxidation state +3 solubility limit in Salado brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
29	3403	SOLMOD4-SOLCIM	Oxidation state +4 solubility limit in Castile brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
30	3407	SOLMOD4-SOLSIM	Oxidation state +4 solubility limit in Salado brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
31	3404	SOLMOD5-SOLCIM	Oxidation state +5 solubility limit in Castile brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
32	3408	SOLMOD5-SOLSIM	Oxidation state +5 solubility limit in Salado brine	Change required for PAVT in 4/25 letter	Use corrected model and new mineral phase (hydromagnesite)
33	3311	AM-PROPMIC	Microbial colloid proportionality constant for americium	Removed in 4/25 letter	Not sensitive
34	3482	AM+3-MKD_AM	Matrix partition coefficient for americium +3	Change required for PAVT in 4/25 letter	Documentation provided and accepted after review
35	3480	PU+3-MKD_PU	Matrix partition coefficient for plutonium +3	Change required for PAVT in 4/25 letter	Documentation provided and accepted after review
36	3481	PU+4-MKD_PU	Matrix partition coefficient for plutonium +4	Change required for PAVT in 4/25 letter	Documentation provided and accepted after review
37	3479	U+4-MKD_U	Matrix partition coefficient for uranium +4	Change required for PAVT in 4/25 letter	Documentation provided and accepted after review
38	3475	U+6-MKD_U	Matrix partition coefficient for uranium +6	Change required for PAVT in 4/25 letter	Documentation provided and accepted after review

No.	ID No.	Material ID - Parameter ID	Description	Disposition	Reason
39	656	WAS_AREA-GRATMICH	Gas generation rate due to microbial action under humid conditions	Removed in 4/25 letter	No sensitivity
40	657	WAS_AREA-GRATMICI	Gas generation rate due to microbial action under inundated conditions	Removed in 4/25 letter	No sensitivity

Table 6.4. Parameters Changed by EPA in Performance Assessment Verification Test

ID No.	Material ID - Parameter ID	Use	Distribution	Minimum	Maximum	Median	Units
198	DRZ_1 - PRMX_LOG ◊	PAVT CCA	Uniform Constant	-19.4 -15.0	-12.5 -15.0	-15.95 -15.0	Log m^2 Log m^2
3184	BH_SAND - PRMX_LOG ◊	PAVT CCA	Uniform Uniform	-16.3 -14.0	-11.0 -11.0	-13.65 -12.5	Log m^2 Log m^2
3185	CONC_PLG - PRMX_LOG ◊	PAVT CCA	Uniform Constant	-19 -16.3	-17 -16.3	-17.3 -16.3	Log m^2 Log m^2
663	WAS_AREA - PRMX_LOG*◊	PAVT CCA	Constant Constant	-12.6198 -12.769	-12.6198 -12.769	-12.6198 -12.769	Log m^2 Log m^2
2131	REPOSIT - PRMX_LOG*◊	PAVT CCA	Constant Constant	-12.6198 -12.769	-12.6198 -12.769	-12.6198 -12.769	Log m^2 Log m^2
2907	STEEL - CORRMCO2	PAVT CCA	Uniform Uniform	0.0 0.0	3.17 E-14 1.59 E-14	1.58 E-14 7.94 E-14	m/s m/s
61	CASTILER - COMP_RCK	PAVT CCA	Triangular Triangular	2.0 E-11 5.0 E-12	1.0 E-10 1.0 E-08	4.0 E-11⌂ 1.0 E-10⌂	Pa^{-1} Pa^{-1}
8000	CASTILER - POR_BPKT ☆	PAVT CCA	Triangular - -	0.1848 - -	0.9240 - -	0.3696⌂ - -	Dimension- less
3493	GLOBAL - PBRINE	PAVT CCA	Uniform Constant	0.01 0.08	0.60 0.08	0.305 0.08	Dimension- less
27	BOREHOLE - DOMEGA	PAVT CCA	Cumulative Constant	4.20 7.8	23.0 7.8	7.8 7.8	Radians/sec Radians/sec
2254	BOREHOLE - TAUFAIL	PAVT CCA	Loguniform Uniform	0.05 0.05	77.0 10.0	2.0 5.025	Pa Pa
3482	AM+3 - MKD_AM	PAVT CCA	Loguniform Uniform	0.02 0.02	0.50 0.50	0.10 0.26	m^3/kg m^3/kg
3480	PU+3 - MKD_PU	PAVT CCA	Loguniform Uniform	0.02 0.02	0.50 0.50	0.10 0.26	m^3/kg m^3/kg
3481	PU+4 - MKD_PU	PAVT CCA	Loguniform Uniform	0.900 0.900	20.0 20.0	4.243 10.45	m^3/kg m^3/kg
3479	U+4 - MKD_U	PAVT CCA	Loguniform Uniform	0.900 0.900	20.0 20.0	4.243 10.45	m^3/kg m^3/kg
3475	U+6 - MKD_U	PAVT CCA	Loguniform Uniform	3.00 E-05 3.00 E-05	3.00 E-02 3.00 E-02	9.49 E-04 1.50 E-02	m^3/kg m^3/kg
3478	TH+4 - MKD_TH	PAVT CCA	Loguniform Uniform	0.900 0.900	20.0 20.0	4.243 10.45	m^3/kg m^3/kg

ID No.	Material ID - Parameter ID	Use	Distribution	Minimum	Maximum	Median	Units
3406	SOLMOD3 - SOLSIM	PAVT CCA	Constant Constant	1.2 E-07 5.82 E-08	1.2 E-07 5.82 E-08	1.2 E-07 5.82 E-08	moles/liter moles/liter
3402	SOLMOD3 - SOLCIM	PAVT CCA	Constant Constant	1.3 E-08 6.52 E-08	1.3 E-08 6.52 E-08	1.3 E-08 6.52 E-08	moles/liter moles/liter
3407	SOLMOD4 - SOLSIM	PAVT CCA	Constant Constant	1.3 E-08 4.4 E-06	1.3 E-08 4.4 E-06	1.3 E-08 4.4 E-06	moles/liter moles/liter
3403	SOLMOD4 - SOLCIM	PAVT CCA	Constant Constant	4.1 E-08 6.0 E-09	4.1 E-08 6.0 E-09	4.1 E-08 6.0 E-09	moles/liter moles/liter
3408	SOLMOD5 - SOLSIM	PAVT CCA	Constant Constant	2.4 E-07 2.3 E-06	2.4 E-07 2.3 E-06	2.4 E-07 2.3 E-06	moles/liter moles/liter
3404	SOLMOD5 - SOLCIM	PAVT CCA	Constant Constant	4.8 E-07 2.2 E-06	4.8 E-07 2.2 E-06	4.8 E-07 2.2 E-06	moles/liter moles/liter

* These parameters replaced BLOWOUT - APORO, which is not used in a current PA code
⌂ This is the mode of the triangular distribution
◊ Parameter similarly varied in Y- and Z-directions
☆ New parameter and number created by DOE for the PAVT to allow brine pocket volume to be varied

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