Sandia National Laboratories

Albuquerque, New Mexico 87185-1341

date: March 27, 1996

to: SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1:
PDD:QA:DISSOLVED SPECIES:Oxidation State
Distribution:Actinides:OX3:OX4:OX5:OX6 (WPO#35194)

from: Ruth Weiner, MS 1341 (6751)

Subject: DISSOLVED SPECIES PARAMETER PRINCIPAL INVESTIGATOR
DOCUMENTATION PACKAGE FOR:OXIDATION STATE
DISTRIBUTION OF ACTINIDES IN THE REPOSITORY

The attached record package contains the oxidation state distribution of the actinide elements thorium, uranium, neptunium, plutonium, americium, and curium in the repository.

The parameter information provided in this record package was collected by Principal Investigators at Sandia National Laboratories for input to the WIPP Data Entry Form and for use by Performance Assessment personnel making parameter estimates. The records package was prepared in accordance with WIPP Quality Assurance Procedure (QAP) 17-1, Rev. 1, WIPP QA Records Source Requirements.

Please call me at 848-0051 if you have any questions.

Exceptional Service in the National Interest

RECORD PACKAGE

DISSOLVED SPECIES PARAMETER PRINCIPAL INVESTIGATOR DOCUMENTATION PACKAGE FOR:

OXIDATION STATE DISTRIBUTION FOR THE ACTINIDE SOURCE TERM

<u>Purpose:</u>   The parameter information provided in this record package was collected by Principal Investigators at Sandia National Laboratories for input to the WIPP Data Entry Form and for use by Performance Assessment personnel making parameter estimates.

<u>Date of Record:</u>   March 27, 1996

<u>Author/Organization</u>: Ruth F. Weiner
                SNL Department 6751
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<u>Recipient:</u>   SWCF-A: Records Center

<u>File Code:</u>   SWCF-A: SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation State Distribution:Actinides:OX3:OX4:OX5:OX6 (WPO#35194)

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation State Distribution:Actinides:OX3:OX4:OX5:OX6

1

RECORD PACKAGE

DISSOLVED SPECIES PARAMETER PRINCIPAL INVESTIGATOR DOCUMENTATION PACKAGE FOR:

OXIDATION STATE DISTRIBUTION FOR THE ACTINIDE SOURCE TERM

SWCF-A: SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation State
Distribution:Actinides:OX3:OX4:OX5:OX6 (WPO#35194)

TABLE OF CONTENTS

Record Number	Contents	Number of Pages
1	Dissolved Species Parameters Required for NUTS and GRIDFLOW	0
2	Attachment 1. *Analysis of Actinide Oxidation States in the WIPP*	40
3	General Correspondence	0
4	Technical Review of Record Package	0
5	Roadmap to Supporting Documentation	2
	TOTAL	0

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation
State Distribution:Actinides:OX3:OX4:OX5:OX6

2

DISSOLVED SPECIES PARAMETERS REQUIRED FOR NUTS AND GRIDFLOW

OXIDATION STATE DISTRIBUTION FOR THE ACTINIDE SOURCE TERM

Prepared by: Ruth F. Weiner, Sandia National Laboratories Department 6751, (505)848-0051, MS 1341

Purpose: The data in this package was collected by Principle Investigators for input to the WIPP Data Entry Form and for use by Performance Assessment personnel making parameter estimates.

I, II.   DATA/PARAMETER

The parameters are the oxidation states of the actinide elements in the repository.

III.   PARAMETER ID

The parameter identifications (IDPRAM) are:

        OX3: oxidation state +3,
        OX4: oxidation state +4
        OX5: oxidation state +5,
        OX6: oxidation state +6

IV, V. MATERIAL ID

The material identifications (IDMTRL) are the symbols usually used to identify the respective actinide elements: thorium (TH), uranium(U), neptunium (NP), plutonium (PU), americium (AM) and curium (CM).

VI.   UNITS

The parameters are unitless.

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation State Distribution:Actinides:OX3:OX4:OX5:OX6

VII. DISTRIBUTION INFORMATION

The parameter value for each material is given in Table 1. The values in the table are the give the oxidation state distribution for each actinide according to the equation:

$$sol_{An} = (OX3)(sol_{An+3}) + (OX4)(sol_{An+4}) + (OX5)(sol_{An+5}) + (OX6)(sol_{An+6})$$

$$sol_{An} = \sum_j (OXj)(sol_{An+j})$$

where sol_{An} is the solubility of the actinide, and sol_{An+j} is the solubility of the +j oxidation state of the actinide.

Table 1.

IDMTRL	IDPRAM			
	OX3	OX4	OX5	OX6
TH	0	1	0	0
U	0	1	0	1
NP	0	1	1	0
PU	1	1	0	0
AM	1	0	0	0
CM	1	0	0	0

A.   CATEGORY

1.   Thorium (TH)

Constant: OX3 = 0
             OX4 = 1
             OX5 = 0
             OX6 = 0

2.   Uranium (U)

Constant: OX3 = 0
             OX4 = 1
             OX5 = 0
             OX6 = 1

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation State Distribution:Actinides:OX3:OX4:OX5:OX6

4

3.   <u>Neptunium</u> (NP)

Constant: OX3 = 0
             OX4 = 1
             OX5 = 1
             OX6 = 0

4.   <u>Plutonium</u> (PU)

Constant: OX3 = 1
             OX4 = 1
             OX5 = 0
             OX6 = 0

5.   <u>Americium</u> (AM)

Constant: OX3 = 1
             OX4 = 0
             OX5 = 0
             OX6 = 0

6.   <u>Curium</u> (CM)

Constant: OX3 = 1
             OX4 = 0
             OX5 = 0
             OX6 = 0

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation
State Distribution:Actinides:OX3:OX4:OX5:OX6

5

VIII. DATA COLLECTION AND INTERPRETATION INFORMATION

A. DATA SOURCES

1. WIPP Observational Data

Data was provided in monthly reports from David Clark (LANL) under SNL Contract AP2274, Linfeng Rao (PNNL) under SNL Contract AP2275, and Donald Reed (ANL-E) under SNL Contract AP2267. These data were all developed under quality assurance (QA) plans approved under the SNL QA program, Rev. R. Data were collected under approved test plans and analyzed under WIPP Analysis Plan AP-AST-01. A summary analysis of these data is given in Attachment 1: *Analysis of Actinide Oxidation States in the WIPP.*

2. Non-WIPP Literature Data

An extensive bibliography is given in Attachment 1. Additional bibliographic information is provided in the *Summary of Literature Solubility Studies* by A. R. Felmy and D. Rai, submitted as a record to meet WIPP Milestone AC059.

B. DATA COLLECTION (FOR WIPP OBSERVATIONAL DATA)

Data collection was performed under the contracts listed below.

1. Contract number: AP 2274

PI name: Ruth F. Weiner (Sandia National Laboratories)
             David L. Clark (Los Alamos National Laboratory)

Approved Test Plan under which data was collected:

Oxidation State Distribution in STTP LANL Document CST-OSD-TST1-002/0 and *Actinide Redox Reactions Important to the WIPP Site,* LANL Document CST-ARR -TST1-003/0, approved 9/5/95. The Test Plan conforms to the requirements of SNL QAP 20-1 with respect to data quality objectives, measurement errors, accuracy and precision, and description of experimental methods, measurements, and testing equipment.

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation State Distribution:Actinides:OX3:OX4:OX5:OX6

6

a. Are all the data qualified: Yes. The February 16, 1996 audit (see c, below) found all the data qualified.

b. Was data qualified by QAP 20-3: No.

c. Was the data the subject of audit/surveillance by SNL or DOE:

The contract was audited by SNL on February 16-18, 1996 (SNL Audit EA 96-12). Four corrective action requests (CARs) were issued, which were closed out on March 25,1996. None of these CARs dealt with data quality.

c. Was the data collected under an SNL approved QA Program: Yes. The LANL QAPjP is *Oxidation State Distribution QAPjP*, LANL Document CST-OSD-QAP1-001/0, approved 9/5/95.

2. Contract number: AP 2275

PI name: Ruth F. Weiner (Sandia National Laboratories)
             Andrew R. Felmy (Pacific Northwest National Laboratory)

Approved Test Plan under which data was collected:

Actinide Redox Reactions Important to the WIPP Site, LANL Document CST-ARR -TST1-003/0, approved 9/5/95. The Test Plan conforms to the requirements of SNL QAP 20-1 with respect to data quality objectives, measurement errors, accuracy and precision, and description of experimental methods, measurements, and testing equipment.

a. Are all the data qualified: Yes.

b. Was data qualified by QAP 20-3: No.

c. Was the data the subject of audit/surveillance by SNL or DOE:

The SNL PI was the subject of a SNL surveillance March 6-7, 1996. The contract is scheduled for a SNL audit on April 23-26, 1996.

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation State Distribution:Actinides:OX3:OX4:OX5:OX6

7

d. Was the data collected under an SNL approved QA Program: Yes. The data was collected under PNNL QA Plan EESD-001, Rev. 0.

2. Contract number: AP 2267

PI name: Robert C. Moore (Sandia National Laboratories)
            Donald T. Reed (Argonne National Laboratory -- East)

Test Plan under which data was collected:

Test Plan for the WIPP Empirical Actinide Stability/Solubility Project, SNL Document. The Test Plan conforms to the requirements of SNL QAP 20-1 with respect to data quality objectives, measurement errors, accuracy and precision, and description of experimental methods, measurements, and testing equipment.

a. Are all the data qualified: Yes.

b. Was data qualified by QAP 20-3: No.

c. Was the data the subject of audit/surveillance by SNL or DOE:

The SNL PI was the subject of a SNL surveillance March 6-7, 1996. The contract is scheduled for a SNL audit on April 23-25, 1996.

d. Was the data collected under an SNL approved QA Program: Yes. The data was collected under QA Plan SNL-SOL-02-002, approved under the SNL QA Plan Rev. R.

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation State Distribution:Actinides:OX3:OX4:OX5:OX6

8

C. INTERPRETATION OF DATA

<u>1. Was the interpretation made by reference to previous work</u>: Yes. An extensive bibliography is given in Attachment 1.

<u>2. Was the interpretation made by using newly performed calculations:</u> No.

<u>3. Form of Interpreted Data</u>: Tables 1 and 2, Section VII.

<u>4. Assumptions Made During Interpretation:</u> The governing assumption is that the chemically reducing environment that resulted in observations of the chemical reduction and consequent disappearance of Pu(VI) and Pu(V) will be the chemical environment in the WIPP. This assumption is consistent with all other WIPP documentation and project positions. Detailed assumptions are discussed in Attachment 1.

<u>5. Name of Code(s)/Software used to Interpret Data:</u> N/A

<u>6. QA Status of Code(s) used to Interpret Data:</u> N/A

<u>7. References Related to Data Interpretation:</u> Attachment 1: *Analysis of Actinide Oxidation States in the WIPP*

<u>8. For interpretations made by using newly performed calculations provide documentation that you followed the requirements of QAP 9-1 Appendix B:</u> N/A

<u>9. For routine calculations (not using code) did you follow requirements of QAP 9-5</u>: N/A

IX. CORRELATION WITH OTHER PARAMETERS:

Oxidation state distribution is correlated with oxidation state solubility for input into NUTS and GRIDFLOW.

X. LIMITATIONS OR QUALIFICATIONS FOR USAGE OF DATA BY PERFORMANCE ASSESSMENT (PA): None.

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA: DISSOLVED SPECIES: Oxidation State Distribution:Actinides:OX3:OX4:OX5:OX6

9

XI.   ATTACHMENTS

Attachment 1: Weiner, R. F., Hobart, D. E., Tait, C. D. and Clark, D. L. *Analysis of Actinide Oxidation States in the WIPP*

RECORD 2

ATTACHMENTS

<u>Attachment 1:</u> Weiner, R. F., Hobart, D. E., Tait, C. D. and Clark, D. L. *Analysis of Actinide Oxidation States in the WIPP*

RECORD 3

GENERAL CORRESPONDENCE

Albuquerque, New Mexico 87185-1341

date: 3/27/96

to: Mary-Alena Martell, Christine Stockman

from: Ruth F. Weiner

subject: Oxidation state distribution of actinides

The parameters for the oxidation state distribution for each element
during the calculation of solutbilities of Th, U, Np, Pu, Am, and Cm
in the CCA NUTS and GRIDFLOW calculations are:

Thorium: TH OX4

Uranium: U OX4, OX6

Neptunium: NP OX4, OX5

Plutonium: PU OX3, OX4

Americium: AM OX3

Curium: CM OX3

cc: R. Vann Bynum
        E. J. Nowak
        Craig F. Novak
        John T. Holmes
        Richard E. Thompson
        SWCF-A: WBS1.1.10.1.1:QA:AST:oxidation state
distribution

SWCF-A: Records Center, SWCF-A:WBS 1.1.10.1.1: PDD:QA:DISSOLVED SPECIES:Oxidation
State Distribution:Actinides:OX3:OX4:OX5:OX6

RECORD 4

Technical Review of Record Package

Salado Parameter Principal Investigator Documentation for:
Actinide Oxidation State Distribution

Technical Review Status:

Scientific Notebooks:
Not Applicable_____; Incomplete___3/27/96_____; Complete_____
                                          (give date)   (give date)

Interpretive Analyses:
Not Applicable_____; Incomplete_____; Complete__3/27/96__
                                          (give date)   (give date)

Routine Calculations:
Not Applicable___x___; Incomplete_____; Complete_____
                                          (give date)   (give date)

Qualification Status:

Data:
Not Applicable_____; Incomplete_____; Complete__2/18/96
                                          (give date)   (give date)

Codes:
Not Applicable___x___; Incomplete_____; Complete_____
                                          (give date)   (give date)

PARAMETER QUALIFIED: Incomplete_____; Complete__2/18/96_____
                                        (give date)   (give date)

RECORD 5

ROADMAP TO SUPPORTING DOCUMENTATION

A. Home Base for this Roadmap

SWCF-A:WBS 1.1.10.1.1: PDD:QA:DISSOLVED SPECIES: Oxidation State Distribution:Actinides:OX3:OX4:OX5:OX6 (WPO#35194)

B. Record Packages that Support the Home Base Package

1. Raw Data Package(s)

_____N/A_____	_N/A__
Title	WPO#

2. Quality Assurance Records

Title	WPO#

C. Record Packages that Depend on the Home Base Package for Support

1. WIPP Data Entry Forms (#464s)

Title	WPO#

Title	WPO#

Title	WPO#

Title	WPO#

2. All inclusive set of WIPP Data Entry Forms (#464) with supporting PA documentation

Title	WPO#

3. Performance Assessment Parameter Database

_____
Title   WPO#

D. Record Packages Collateral to the Home Base Package

1. Other PI/SI Record Package(s) for the same idmtrl/idpram as the Home Base Record Package

__Documentation for Milestone AC055 (WBS 1.1.10.1.1), SWCF-A: WBS 1.1.10.1.1:AST:QA:oxidation state_, no WPO#._____

__Documentation for Milestone AC056 (WBS 1.1.10.1.1), SWCF-A: WBS 1.1.10.1.1:AST:QA:oxidation state_, no WPO#._____

__Documentation for Milestone AC058 (WBS 1.1.10.1.1), SWCF-A: WBS 1.1.10.1.1:AST:QA:oxidation state_, no WPO#._____

__Documentation for Milestone AC059 (WBS 1.1.10.1.1), SWCF-A: WBS 1.1.10.1.1:AST:QA:oxidation state_, no WPO#._____

__Documentation for Milestone AC080 (WBS 1.1.10.1.1), SWCF-A: WBS 1.1.10.1.1:AST:QA:oxidation state_, no WPO#._____

2. Performance Assessment (PA) Record Package pertaining to dispute resolution

_____N/A_____N/A__
Title   WPO#