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**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*

SWCF-A: WBS 1.1.10.1.1: PDD:QA:DISSOLVED SPECIES: OXIDATION STATE DISTRIBUTION:  
ACTINIDES:OX3:OX4:OX5:OX6

Information Only

## RECORD PACKAGE

### DISSOLVED SPECIES PARAMETER PRINCIPAL INVESTIGATOR DOCUMENTATION PACKAGE FOR:

#### OXIDATION STATE DISTRIBUTION FOR THE ACTINIDE SOURCE TERM

Purpose: 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.

Date of Record: March 27, 1996

Author/Organization: Ruth F. Weiner  
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Recipient: SWCF-A: Records Center

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

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

Information Only

## 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)

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

Information Only

## RECORD 1

### 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.

## VII. DISTRIBUTION INFORMATION

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

$$\text{sol}_{\text{An}} = (\text{OX3})(\text{sol}_{\text{An}+3}) + (\text{OX4})(\text{sol}_{\text{An}+4}) + (\text{OX5})(\text{sol}_{\text{An}+5}) + (\text{OX6})(\text{sol}_{\text{An}+6})$$

$$\text{sol}_{\text{An}} = \sum_j (\text{OXj})(\text{sol}_{\text{An}+j})$$

where  $\text{sol}_{\text{An}}$  is the solubility of the actinide, and  $\text{sol}_{\text{An}+j}$  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

3. Neptunium (NP)

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

4. Plutonium (PU)

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

5. Americium (AM)

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

6. Curium (CM)

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

## 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.

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.



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.

## C. INTERPRETATION OF DATA

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

2. Was the interpretation made by using newly performed calculations: No.

3. Form of Interpreted Data: Tables 1 and 2, Section VII.

4. Assumptions Made During Interpretation: 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.

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

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

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

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

9. For routine calculations (not using code) did you follow requirements of QAP 9-5: 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.

## 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**

Attachment 1: 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**

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

**Information Only**

Sandia National Laboratories

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 solubilities 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 *RVB*  
E. J. Nowak *EJN*  
Craig F. Novak  
John T. Holmes  
Richard E. Thompson  
SWCF-A: WBS1.1.10.1.1:QA:AST:oxidation state  
distribution

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)

Title	WPO#
N/A	N/A

2. Quality Assurance Records

Title	WPO#
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**C. Record Packages that Depend on the Home Base Package for Support**

1. WIPP Data Entry Forms (#464s)

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

Title	WPO#
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### 3. Performance Assessment Parameter Database

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Title	WPO#
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#### 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

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N/A	N/A
Title	WPO#