Estimate of Complexing Agents in TRU Waste for The Compliance Recertification Application

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August 26, 2003

Author — Beverly A. Crawford — 8/27/03
Beverly Crawford, EES-12 — Date
LANL Carlsbad Operations

Author — 8/27/03
Christi Leigh, 6821 — Date
SNL Performance Assessment and Decision Analysis Group

Technical Review — 8/27/03
Laurie Sparks-Roybal, EES-12 — Date
LANL Carlsbad Operations

QA Review — Kathleen Byle — 8-28-03
Kathleen Byle — Date
SNL Carlsbad Programs Group

Management Review — 8/27/03
David Kessel, 6821 — Date
SNL Performance Assessment and Decision Analysis Manager

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1. INTRODUCTION

In 1996 the Department of Energy (DOE) completed a performance assessment (PA) calculation for the Waste Isolation Pilot Plant (WIPP). The PA was part of the Compliance Certification Application (CCA) submitted to the Environmental Protection Agency (EPA) to demonstrate compliance with the radiation protection regulations of 40 Code of Federal Regulations (CFR) 191 and 40 CFR 194. As required by the WIPP Land Withdrawal Act (U.S. DOE and State of New Mexico, 1981), DOE is required to submit documentation to EPA for the recertification of the WIPP every five years in order to continue operating the site. This will require that a Compliance Recertification Application (CRA) be prepared and submitted to the EPA by November 2003.

This analysis is governed by AP-092, *Analysis Plan for Transuranic Waste Inventory Update Report, 2003.* In particular, an estimate of the mass of complexing agents (acetic acid, sodium acetate, citric acid, sodium citrate, oxalic acid, sodium oxalate, and sodium EDTA) that are destined for disposal in the WIPP repository based on updated inventory information collected by Los Alamos National Laboratories – Carlsbad Office (LANL-CO) is required. This information is then used in PA determinations to support the CRA. This analysis was performed in accordance with the Sandia National Laboratories (SNL) Quality Assurance Program and was prepared as prescribed by the SNL NWMP Procedure, NP 9-1, *Analyses.*

1.1 ACRONYMS

AP	Analysis Plan
CCA	Compliance Certification Application
CFR	Code of Federal Regulations
CRA	Compliance Recertification Application
DOE	Department of Energy
EDTA	Ethylenediaminetetraacetic Acid
EPA	Environmental Protection Agency
ERMS	Electronic Records Management System
LANL	Los Alamos National Laboratory
LANL-CO	Los Alamos National Laboratory – Carlsbad Office
NP	NWMP Procedure
NWMP	Nuclear Waste Management Program
PA	Performance Assessment
RFETS	Rocky Flats Environmental Technology Site
RP	Hanford Office of River Protection
SNL	Sandia National Laboratories
TRU	Transuranic
TWBIR	Transuranic Waste Baseline Inventory Report
TWBID	Transuranic Waste Baseline Inventory Database
WIPP	Waste Isolation Pilot Plant

2. PROBLEM DESCRIPTION

In support of the WIPP PA for the CCA, the DOE prepared the *Waste Isolation Pilot Plant Transuranic Waste Baseline Inventory Report, Revision 3* (U.S. DOE 1996a) which is referred to throughout the rest of this document as the TWBIR Revision 3. The purpose of the TWBIR Revision 3 was to document the total inventory of DOE TRU waste.

In support of the CRA, the DOE is preparing the *Transuranic Waste Inventory Update Report, 2003*. The purpose of the *Transuranic Waste Inventory Update Report, 2003* is to update the total inventory of DOE TRU waste for recertification of the WIPP repository. Therefore, DOE through its contractor, LANL-CO, issued a data call to the generator sites. Data collected during the 2003 update data call has been processed and is currently stored in the Transuranic Waste Baseline Inventory Database (TWBID) Revision 2.1, Version 3.12, Data Version D.4.08, developed by LANL-CO (LANL 2003a) and in hard copy record at the SNL WIPP Records Center. TWBID Revision 2.1 Version 3.12 was qualified in accordance with NP 19-1, *Software Requirements,* and is the source of data for this calculation.

Scaled waste stream volumes for waste emplaced in the WIPP repository and waste coming to the WIPP repository from the generator sites for the *Transuranic Waste Inventory Update Report, 2003* have been provided by LANL (LANL 2003b). The scaled volume is the inventory volume defined for WIPP emplacement to be used for PA calculations for the CRA. The Land Withdrawal Act defines the total amount of TRU waste allowed in the WIPP as 6,200,000 ft^3 or 175,538 m^3 (U.S. Congress, 1992). The "Agreement for Consultation and Cooperation" limits the RH TRU inventory to 250,000 ft^3 (U.S. DOE and State of New Mexico, 1981). By difference, the CH TRU inventory is limited to 5,950,000 ft^3.

The PA for the CRA requires an estimate of the mass of complexing agents expected for disposal in the repository. An estimate of the mass of complexing agents expected for disposal for the CCA was given in Appendix B-4 of the TWBIR Revision 3. The purpose of this calculation is to estimate the total mass of complexing agents expected in the scaled waste stream volumes reported for the update in support of the WIPP CRA PA .

3. ANALYSIS

This calculation is based on data obtained from Appendix B-4 of the TWBIR Revision 3 and data updates provided for the *Transuranic Waste Inventory Update Report, 2003*. Appendix B-4 of the TWBIR Revision 3 reported the complexing agents for TRU solidified waste forms scheduled for disposal in WIPP. Several complexing agents were identified in waste reported in Appendix B-4. However, only two sites, Rocky Flats Environmental Technology Site (RFETS) and Los Alamos National Laboratory (LANL) provided data on acetic acid, sodium acetate, citric acid, sodium citrate, oxalic acid, sodium oxalate, and sodium EDTA in the TWBIR Revision 3. Data from Table 3 of Appendix B-4 from the TWBIR Revision 3 is shown in Table 1. RFETS reported additional EDTA in waste stream RF-MT-0541 (LANL 2003c) and the Hanford Office of River Protection (Hanford-RP) identified sodium acetate and sodium oxalate in three waste streams generated from tank farm wastes in their recent data updates (LANL 2003d).

Table 1. Complexing Agent Masses for Waste Streams Reported in the TWBIR Revision 3[a]

Complexing Agent	RFETS	LANL[c]	Hanford[b]	Total
Acetic Acid	132	10	---	142
Sodium Acetate	1,110	---	---	1,110
Citric Acid	90	1,100.5	---	1,190.5
Sodium Citrate	400	---	---	400
Oxalic Acid	90	13,706		13,796
Sodium Oxalate	----	---	---	---
EDTA	23	---	---	23

[a]From Table 3 Appendix B-4 of the TWBIR Revision 3; [b]At the time of the TWBIR Revision 3, Hanford was only the Hanford Richland Office. Now Hanford also includes the Hanford Office of River Protection; [c]While the memoranda concerning complexing agents in TRU waste addressed to Paul Drez from LANL at the time of the TWBIR Revision 3 do not specify whether the complexing agents contained in LANL waste streams are in the acid form or in the form of sodium salts, Table 3 of Appendix B-4 indicates that the compounds are in the acid form. That assumption is maintained in this document.

3.1 LANL COMPLEXING AGENTS

LANL reported an inventory of complexing agents by technical area and waste description in the submission for the TWBIR Revision 3. The waste identified at LANL as containing complexing agents for the TWBIR Revision 3 is summarized in Table 2. The waste included Technical Area 55 cemented evaporator bottoms (S3000 homogeneous solids), Technical Area 50 dewatered sludges (S3000 homogeneous solids), and Technical Area 55 combustible wastes (S5000 heterogeneous debris waste). The quantities of acetic acid, sodium acetate, citric acid, sodium citrate, oxalic acid, sodium oxalate, and sodium EDTA for these waste streams are shown in Table 1. While the memoranda concerning complexing agents in TRU waste addressed to Paul Drez from LANL at the time of the TWBIR Revision 3 do not specify whether the complexing agents contained in LANL waste streams are in the acid form or in the form of sodium salts, Table 3 of Appendix B-4 indicates that the compounds are in the acid form. That assumption is maintained in this document. No additional data was added in the recent data call in support of the *Transuranic Waste Inventory Update Report, 2003.*

Table 2. Complexing Agents in LANL Waste Streams

TWBIR Revision 3 Description
Technical Area 50 - Dewatered sludge from pretreatment and liquid waste
Technical Area 55 -Combustible waste containing rags used in decontamination or spill clean-up
Technical Area 55 – Cemented evaporator bottoms

3.2 RFETS COMPLEXING AGENTS

RFETS reported complexing agents used on site over a twenty-year period based on procurement estimates in the TWBIR Revision 3 (see Appendix B-4 Table 3 in DOE 1996a). That inventory is shown in Table 1. Complexing agents were known to be used in generation of saltcrete waste

at RFETS. No other TRU waste processes that use complexing agents were identified for the TWBIR Revision 3 (DOE 1996a). The authors of the TWBIR Revision 3 note that assigning the entire procured mass of these chemicals (acetic acid, sodium acetate, citric acid, sodium citrate, oxalic acid, sodium oxalate, and sodium EDTA) to the TRU waste stream is a very conservative assumption. However, RFETS did not provide any further information about the consumption of of acetic acid, sodium acetate, citric acid, sodium citrate, oxalic acid, sodium oxalate, and sodium EDTA in processes at the site. Therefore, for the CRA, it is assumed that the entire procured mass of acetic acid, sodium acetate, citric acid, sodium citrate, oxalic acid, sodium oxalate, and sodium EDTA exists in the TRU waste stream coming to WIPP from RFETS.

During the recent data call in support of the *Transuranic Waste Inventory Update Report, 2003*, RFETS reported an additional waste stream, RF-MT0541, that contains EDTA. The amount of EDTA that was reported by the site in the RF-MT0541 waste stream (LANL 2003c) indicated that less than 1 weight percent of the waste stream was EDTA. The material density for this waste stream is 59.0 kg/m^3 (LANL 2003a) and the waste stream volume is 4.38 m^3(LANL 2003b). The mass of the waste stream is 258.42 kg (density times volume). Therefore, the maximum EDTA content is 2.58 kg (.01 times the waste stream mass).

3.3 HANFORD OFFICE OF RIVER PROTECTION COMPLEXING AGENTS

In the recent data call in support of the *Transuranic Waste Inventory Update Report, 2003*, Hanford-RP reported three waste streams that contain complexing agents. A summary of the complexing agents reported for those waste streams (LANL 2003d) is given in Table 3.

Table 3. Complexing Agents Reported for Hanford-RP Waste Streams[a]

Waste Stream	Complexing Agent	Complexing Agent Mass Reported (kg)
RP-W013	Sodium Oxalate	26,000.0
RP-W016	Sodium Acetate	7,400.0
	Sodium Oxalate	6,490.0
RP-W754	Sodium Oxalate	1,450.0

[a]Source is LANL 2003d

3.4 TOTAL MASS OF COMPLEXING AGENTS

The total mass of all complexing agents requested by SNL (Giambalvo 2002a and b) is calculated by summing the masses from Table 1, the additional EDTA mass from RFETS and the additional sodium oxalate and sodium acetate masses from Hanford-RP. These totals are shown in Table 4).

Table 4. Total Mass of Complexing Agents In The WIPP Repository For The CRA

Complexing Agent	RFETS	LANL[c]	Hanford[b]	Total
Acetic Acid	132	10	---	142
Sodium Acetate	1,110	---	7,400	8,510
Citric Acid	90	1,100.5	---	1,190.5
Sodium Citrate	400	---	---	400
Oxalic Acid	90	13,706	---	13,796
Sodium Oxalate	----	---	33,940	33,940
EDTA	25.6	---	---	25.6

4. RESULTS

The total mass of complexing agents for each site are reported in Table 4. Table 4 also provides the total complexing agents for the repository based on the updated quantities and those reported in the TWBIR Revision 3. Large contributions of the sodium salts of oxalate and acetate originated from the Hanford-RP waste. This waste was not included in the TWBIR Revision 3. Hanford RP contributed the largest amount of sodium acetate (7400 kg) and the total amount of acetic acid (coming from LANL and RFETS) is 142 kg. Sodium acetate and sodium citrate were also reported by RFETS for the TWBIR Revision 3 and this information has not changed for the *Transuranic Waste Inventory Update Report, 2003*. The total mass of sodium-containing complexing agents is 8,510 kg plus 400 kg plus 33,940, which equals 42,850 kg.

Combustible waste at LANL contains rags used during decontamination and clean-up that contain citric acid. Citric acid was also identified as being generated from some production processes at RFETS. The total contributions from citrate/citric acid are 1,190.5 kg. Large contributions of oxalic acid came from LANL with a smaller amount originating from RFETS (total equals 13,796 kg).

5. RELEVANT PROCEDURES AND REFERENCES

5.1 PROCEDURES

AP-092, "Analysis Plan for Transuranic Waste Inventory Update Report, 2003 " Sandia National Laboratory Nuclear Waste Management Program Analysis Plan, January 8, 2003.

NP 9-1, "Analyses." Sandia National Laboratory Nuclear Waste Management Program Procedure, August 29, 2001.

NP 19-1, "Software Requirements." Sandia National Laboratory Nuclear Waste Management Program Procedure, June 12, 2002.

5.2 REFERENCES

Giambalvo 2002a. Sandia's WIPP Inventory Data Needs for Performance Assessment, Letter to J. Harvill, April 22, 2002, Carlsbad, NM.

Giambalvo 2002b. Waste Inventory: Level of Detail Required for Performance Assessment, Letter to J. Harvill, June 10, 2002, Carlsbad, NM.

LANL 2003a. *Transuranic Waste Baseline Inventory Database, Revision 2.1, Version 3.12.* Software Installation and Checkout Form. ERMS# 530624. Carlsbad, NM: Los Alamos National Laboratory. August 12, 2003.

LANL 2003b. *Response to Request for Radionuclide Activities in TRU Waste Streams from the TWBID Revision 2.1 Version 3.12; Data Version D.4.08.* ERMS#530918. Carlsbad, NM: Los Alamos National Laboratories.

LANL 2003c. *Rocky Flats Environmental Technology Office (RFETS).* Data Package. ERMS# 526779. Carlsbad , NM: Los Alamos National Laboratory. March 25, 2003.

LANL 2003d. *Hanford Office of River Protection (Hanford-RP).* Data Package. ERMS# 526473. Carlsbad , NM: Los Alamos National Laboratory. March 17, 2003.

U.S. Congress 1992. *Waste Isolation Pilot Plant Land Withdrawal Act*, Public Law 102-579, 1992, and amended Public Law 104-201, 1996.

U.S. Department of Energy 1996a. *Waste Isolation Pilot Plant Transuranic Waste Baseline Inventory Report, Revision 3*, DOE/CAO-1996-2184. Carlsbad, NM: U.S. Department of Energy.

U.S. Department of Energy and State of New Mexico 1981. *Agreement for Consultation and Cooperation Between the Department of Energy and the State of New Mexico on the Waste Isolation Pilot Plant*, July 1981 (dated April 18, 1988).

Attachment I : Email Correspondence from RFETS With Data For RF-TT-0541

Beverly A. Crawford 3/28/03

X-XSP-MXS-Processed: 1
X-XSP-EXPP-Processed: 1
Importance: normal
Priority: normal
Subject: RE: Info on RF Waste Streams (FWF, WMC)
Date: Mon, 24 Mar 2003 14:54:02 -0700
X-MS-Has-Attach:
X-MS-TNEF-Correlator:
Thread-Topic: Info on RF Waste Streams (FWF, WMC)
thread-index: AcLyGEmLy47OmRmrRjWYIT1TOlOcMAANLyeQ
From: "Sendelweck, Vivian" <Vivian.Sendelweck@rfets.gov>
To: "Laurie Sparks-Roybal" <sparkie@lanl.gov>
Cc: <crawford@lanl.gov>, <jerrim@lanl.gov>, <slott@lanl.gov>
X-OriginalArrivalTime: 24 Mar 2003 21:54:03.0188 (UTC) FILETIME=
[E23E7F40:01C2F24F]
X-MIME-Autoconverted: from quoted-printable to 8bit by ees-mail.lanl.gov id
h2OLs6l2023149

Laurie:
RFETS agrees with the listings as shown below if the revision is made to RF-TT0541.

Bev:
for IDC 0541 (analytical lab solution)
EDTA - may be present at the T level (Trace Component <1% by wt.)
nitrates, sulfates, and phosphates - may be present at the D level (Dominant Component >10% by wt.) material may have been dissolved in acid as part of analysis.

Liquids will be processed to a solid prior to shipment - any D001, D002, D003 wastes will be treated to remove the prohibited nature of the waste.

Please call if you need clarification or more information.

Vivian S. Sendelweck
Wastren, Inc.
TRU Waste Programs and Projects - Acceptable Knowledge
B460, 222-06

Voice: (303) 966-8278
FAX: (303) 966-2952
Email: vivian.sendelweck@RFETS.gov

> -----Original Message-----
> From: Laurie Sparks-Roybal [SMTP:sparkie@lanl.gov]
> Sent: Monday, March 24, 2003 8:16 AM
> To: Sendelweck, Vivian
> Cc: crawford@lanl.gov; jerrim@lanl.gov; slott@lanl.gov
> Subject: Info on RF Waste Streams (FWF, WMC)
>
> Hi Vivian,
> Thank you for calling this morning. Here is what I have:

>
> RF-MT0503 Not enough information to estimate a FWF/WMC.
> RF-MT0505 Not enough information to estimate a FWF/WMC.
> RF-MT0529 Not enough information to estimate a FWF/WMC.
> RF-MT0533 Not enough information to estimate a FWF/WMC.
> RF-MT0535 Not enough information to estimate a FWF/WMC.
>
> RF-MT0545 The final waste form is "inorganic non-metal." The estimated
> waste matrix code is S3160, Inorganic Chemicals (based on TWBIR Revision 2,
> Table 1-2, and the DOE Waste Treatability Group Guidance).
>
> RF-TT0533 Not enough information to estimate a FWF/WMC.
>
> RF-TT0541 The final waste form reported is "solidified inorganics." The
> estimated waste matrix code is S3125, Reprocessing Sludges S3129, Unknown/Other
Inorganic Sludges (based on TWBIR
> Revision 2, Table 1-2, and the DOE Waste Treatability Group Guidance).
>
> RF-TT0545 The final waste form reported is "inorganic non-metal." The
> estimated waste matrix code is S3160, Inorganic Chemicals (based on TWBIR
> Revision 2, Table 1-2, and the DOE Waste Treatability Group Guidance).
>
> RF-MT0886 The final waste form reported is "solidified inorganics." The
> estimated waste matrix code is S3160, Inorganic Chemicals (based on TWBIR
> Revision 2, Table 1-2, and the DOE Waste Treatability Group Guidance).
>
> RF-MT0971 The final waste form reported is "uncategorized metal." The
> estimated waste matrix code is S5110, Metal Debris (based on TWBIR Revision
> 2, Table 1-2, and the DOE Waste Treatability Group Guidance).
>
> RF-MT0972 The final waste form reported is "heterogeneous." The estimated
> waste matrix code is S5440, Predominantly Organic Debris (based on TWBIR
> Revision 2, Table 1-2, and the DOE Waste Treatability Group Guidance).
>
> RF-MT0973 The final waste form reported is "uncategorized metal." The
> estimated waste matrix code is S5110, Metal Debris (based on TWBIR Revision
> 2, Table 1-2, and the DOE Waste Treatability Group Guidance).
>
> Please let me know if RFETS finds these estimations acceptable. If so, they
> will be entered into the inventory database. We are in the process of
> determining whether it will be necessary to estimate the FWF and WMC for
> the waste streams that have limited information.
> Thank you for your assistance.
>
> Laurie Sparks-Roybal
> Los Alamos National Laboratory
> Earth and Environmental Sciences Division - Carlsbad Operations
> 115 North Main Street
> Carlsbad, NM 88220
> 505-628-3255 office, 505-390-5763 cel

Attachment II: Email Correspondence from Hanford-RP With Complexing Agent Data

Leigh, Christi D

From: Sheila Lott [slott@lanl.gov]
Sent: Wednesday, August 27, 2003 11:12 AM
To: cdleigh@sandia.gov
Subject: Fwd: FW:

8/27/03

From: "Kristofzski, John G" <John_G_Kristofzski@rl.gov>
To: "'Sheila Lott'" <slott@lanl.gov>, "'Beverly Crawford'" <crawford@lanl.gov>
Cc: "Coony, Francis M (Mike)" <Francis_M_Mike_Coony@rl.gov>
Subject: FW:
Date: Mon, 7 Apr 2003 08:20:33 -0700
X-Mailer: Internet Mail Service (5.5.2232.9)
X-RCPT-TO: <131229@empo.lanl.gov>

-----Original Message-----
From: Reddick, George W Jr
Sent: Monday, April 07, 2003 8:02 AM
To: Kristofzski, John G
Cc: Boomer, Kayle D; Mackay, Stewart M; Haigh, Paul G
Subject:

John:

This is the updated information for the TRU streams.

==========

Stream Name: PFP TRU Solids, W-013

Chemical	Value	Units
Sulfate	14,300	kgs
Nitrate	440,000	kgs
Phosphate	18,000	kgs
Acetate		
Citrate		
Oxalate	26,000	kgs
EDTA		
TOC	25,500	kgs

==========

==========

Stream Name: PUREX TRU Cladding Removal Solids, W-016

Chemical	Value	Units
Sulfate	13,500	kgs

Nitrate	505,000	kgs
Phosphate	12,900	kgs
Acetate	7,400	kgs
Citrate		
Oxalate	6,490	kgs
EDTA		
TOC	15,700	kgs

Stream Name: 224 Waste, W-754

Chemical	Value	Units
Sulfate	747	kgs
Nitrate	73,100	kgs
Phosphate	11,200	kgs
Acetate		
Citrate		
Oxalate	1,450	kgs
EDTA		
TOC	1,100	kgs

Stream Name: Bismuth Phosphate TRU Solids, W-755

Chemical	Value	Units
Sulfate	6,860	kgs
Nitrate	122,000	kgs
Phosphate	63,300	kgs
Acetate		
Citrate		
Oxalate		
EDTA		
TOC	7,260	kgs

This information was obtained from the TWINS data. Please let me know if you need additional information.

Thanks
GWR

Sheila Lott
Los Alamos National Laboratory-Carlsbad Operations
EES-12
115 North Main Street

Carlsbad, NM 88220

Phone - 505-628-1372
Cell - 505-706-0224
slott@lanl.gov