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ENGINEERING CHANGE NOTICE

Page 1 of 2

1. ECN 644460

Proj. ECN

2. ECN Category (mark one)	3. Originator's Name, Organization, MSIN, and Telephone No.	4. USQ Required?	5. Date
Supplemental [X] Direct Revision [X] Change ECN [] Temporary [] Standby [] Supersedure [] Cancel/Void []	M.J. Kupfer, LMHC, H5-49 376-6631	[] Yes [X] No	08/26/97
	6. Project Title/No./Work Order No. Tank 241-SX-113	7. Bldg./Sys./Fac. No. NA	8. Approval Designator NA
	9. Document Numbers Changed by this ECN (includes sheet no. and rev.) WHC-SD-WM-ER-480, Rev. 0B	10. Related ECN No(s). NA	11. Related PO No. NA

12a. Modification Work	12b. Work Package No.	12c. Modification Work Complete	12d. Restored to Original Condition (Temp. or Standby ECN only)
[] Yes (fill out Blk. 12b) [X] No (NA Blks. 12b, 12c, 12d)	NA	NA Design Authority/Cog. Engineer Signature & Date	NA Design Authority/Cog. Engineer Signature & Date

13a. Description of Change

13b. Design Baseline Document? [] Yes [X] No

Add Appendix A, Evaluation to Establish Best-Basis Inventory for Single-Shell Tank 241-SX-113.

14a. Justification (mark one)

Criteria Change	[]	Design Improvement	[]	Environmental	[]	Facility Deactivation	[]
As-Found	[X]	Facilitate Const	[]	Const. Error/Omission	[]	Design Error/Omission	[]

14b. Justification Details

An effort is underway to provide waste inventory estimates that will serve as standard characterization source terms for the various waste management activities. As part of this effort, an evaluation of available information for single-shell tank 241-SX-113 was performed, and a best-basis inventory was established. This work follows the methodology that was established by the standard inventory task.

15. Distribution (include name, MSIN, and no. of copies)

Central Files	A3-88	K. M. Hall	R2-12
DOE Reading Room	H2-53	K. M. Hodgson	R2-11
TCSRC	R1-10	R. T. Winward	H5-49
File	H5-49	L. M. Sasaki	R2-12
W. W. Schulz	H5-49		
M. J. Kupfer	H5-49		
M. D. LeClair (3)	H0-50		

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DATE: AUG 28 1997

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ENGINEERING CHANGE NOTICE

1. ECN (use no. from pg. 1) 644460

16. Design Verification Required	17. Cost Impact				18. Schedule Impact (days)	
	ENGINEERING		CONSTRUCTION			
[] Yes	Additional	[] $	Additional	[] $	Improvement	[]
[X] No	Savings	[] $	Savings	[] $	Delay	[]

19. Change Impact Review: Indicate the related documents (other than the engineering documents identified on Side 1) that will be affected by the change described in Block 13. Enter the affected document number in Block 20.

SDD/DD	[]	Seismic/Stress Analysis	[]	Tank Calibration Manual	[]
Functional Design Criteria	[]	Stress/Design Report	[]	Health Physics Procedure	[]
Operating Specification	[]	Interface Control Drawing	[]	Spares Multiple Unit Listing	[]
Criticality Specification	[]	Calibration Procedure	[]	Test Procedures/Specification	[]
Conceptual Design Report	[]	Installation Procedure	[]	Component Index	[]
Equipment Spec.	[]	Maintenance Procedure	[]	ASME Coded Item	[]
Const. Spec.	[]	Engineering Procedure	[]	Human Factor Consideration	[]
Procurement Spec.	[]	Operating Instruction	[]	Computer Software	[]
Vendor Information	[]	Operating Procedure	[]	Electric Circuit Schedule	[]
OM Manual	[]	Operational Safety Requirement	[]	ICRS Procedure	[]
FSAR/SAR	[]	IEFD Drawing	[]	Process Control Manual/Plan	[]
Safety Equipment List	[]	Cell Arrangement Drawing	[]	Process Flow Chart	[]
Radiation Work Permit	[]	Essential Material Specification	[]	Purchase Requisition	[]
Environmental Impact Statement	[]	Fac. Proc. Samp. Schedule	[]	Tickler File	[]
Environmental Report	[]	Inspection Plan	[]		[]
Environmental Permit	[]	Inventory Adjustment Request	[]		[]

20. Other Affected Documents: (NOTE: Documents listed below will not be revised by this ECN.) Signatures below indicate that the signing organization has been notified of other affected documents listed below.

Document Number/Revision	Document Number/Revision	Document Number Revision
NA		

21. Approvals

	Signature	Date		Signature	Date
Design Authority			Design Agent		
Cog. Eng. M. J. Kupfer	M J Kupfer	8-27-97	PE		
Cog. Mgr. K. M. Hodgson	K. M. Hodgson	8-27-97	QA		
QA			Safety		
Safety			Design		
Environ.			Environ.		
Other L. M. Sasaki	RD Akiel for LMS	8/27/97	Other		

DEPARTMENT OF ENERGY

Signature or a Control Number that tracks the Approval Signature

ADDITIONAL

Tank Characterization Report for Single-Shell Tank 241-SX-113

W. W. Schulz (W^2S Company), R. T. Winward (Meier Associates), and M. J. Kupfer
Lockheed Martin Hanford Corporation, Richland, WA 99352
U.S. Department of Energy Contract DE-AC06-96RL13200

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Abstract: An effort is underway to provide waste inventory estimates that will serve as standard characterization source terms for the various waste management activities. As part of this effort, an evaluation of available information for single-shell tank 241-SX-113 was performed, and a best-basis inventory was established. This work follows the methodology that was established by the standard inventory task.

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Christine L. McNeil 8/28/97
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RECORD OF REVISION	(1) Document Number WHC-SD-WM-ER-480	Page 1

(2) Title
Tank Characterization Report for Single-Shell Tank 241-SX-113

CHANGE CONTROL RECORD

(3) Revision	(4) Description of Change - Replace, Add, and Delete Pages	Authorized for Release (5) Cog. Engr.	(6) Cog. Mgr. Date
0	(7) Initially released 08/04/95 on EDT-613107.	J.H. Baldwin	J.G. Kristofzski
0-A RS	Incorporate per ECN-623837.	L.M. Sasaki	J.G. Kristofzski 8/31/95
0-B RS	Incorporate per ECN-625694.	L.M. Sasaki	J.G. Kristofzski
0C RS	Incorporate per ECN 644460	M.J. Kupfer 8-27-97	K.M. Hodgson 8-27-97

APPENDIX A

EVALUATION TO ESTABLISH BEST-BASIS INVENTORY FOR SINGLE-SHELL TANK 241-SX-113

APPENDIX A

EVALUATION TO ESTABLISH BEST-BASIS INVENTORY FOR SINGLE-SHELL TANK 241-SX-113

An effort is underway to provide waste inventory estimates that will serve as standard characterization source terms for the various waste management activities (Hodgson and LeClair 1996). As part of this effort, an evaluation of available information for single-shell tank 241-SX-113 was performed, and a best-basis inventory was established. This work, detailed in the following sections, follows the methodology that was established by the standard inventory task.

A1.0 CHEMICAL INFORMATION SOURCES

This Tank Characterization Report (TCR) for tank 241-SX-113 summarizes the only available sampling event, an auger sampling in May 1995. The sampling and analyses were performed in accordance with the Tank Screening Data Quality Objective (Babad and Redus 1994). Only the total alpha activity, water content, density, and energetics of the augured sample were evaluated. No data were obtained for the content of other radionuclides or nonradioactive chemicals. The density of the solids in tank 241-SX-113 was found to be 1.40 g/cc.

Two samples were collected from tank 241-SX-113 using 50.8-cm (20-in.) augers. Sample 95-AUG-028 was collected from riser 7 and sample 95-AUG-029 was collected from riser 6. Auger sampling was used because the waste material was expected to consist of sludge approximately 38 cm (15 in.) in depth. The 50.8-cm 20-inch augers were expected to recover about 14 cm (5.5 in.) for sample 95-AUG-028 and 17.8 cm (7 in.) for sample 95-AUG-029. Sample 95-AUG-028 had waste material on all flutes of the auger for a total recovery of 249 grams. Most waste material was on the lower half of the auger for sample 95-AUG-029 for a total recovery of 97.8 grams.

In 1996 archived portions of the homogenized auger samples from tank 241-SX-113 were sent to Los Alamos National Laboratory (LANL). Investigators at LANL in the course of conducting sludge washing experiments had occasion to analyze their sample of solids in tank 241-SX-113 for various radioactive and nonradioactive analytes.

The Hanford Defined Waste (HDW) model report (Agnew et al. 1997) provides tank content estimates, derived from the LANL model, in terms of component concentrations and inventories.

Tank 241-SX-113 is a known leaker. However, the quantity of material lost to the soil column is currently unknown. No attempt has been made in this assessment to correct for materials lost to the soil column.

A2.0 COMPARISON OF COMPONENT INVENTORY VALUES

Hanlon (1996) estimates that tank 241-SX-113 contains 98 kL (26 kgal) of sludge; no drainable liquid remains. According to the HDW model, tank 241-SX-113 contains 117 kL (31 kgal) of solids whose water content is 1.81 wt%, the HDW model also lists a value of 0.478 g/cc for the density of the solids in tank 241-SX-113. The latter value is obviously incorrect and likely represents the density of unreacted diatomaceous earth.

Table A2-1 lists the predictions of the HDW model for the inventories of various analytes in tank 241-SX-113 solid waste. The inventory of analytes in the solids in tank 241-SX-113 as determined by direct analysis of such solids (at LANL) is also listed in Table A2-1. (The chemical species are reported without charge designation per the best-basis inventory convention.)

Table A2-1. Comparison of Tank 241-SX-113 Historical Tank Content-Based Inventory Estimates for Selected Analytes with Auger Sample Results. (2 Sheets)

Analyte	HDW model inventory estimate (kg)[a]	Analysis of auger samples[b]
Al	1,660	1,190
Bi	0	0.46
Ca	419	211
Cl	13.8	NR
CO_3	99.7	NR
Cr	24.3	6.34
Fe	979	1,360
K	3.32	76.9
Mn	0	36.6
Na	28,300	95.9
Ni	22.5	0.60
NO_2	507	NR
NO_3	2,480	NR
Pb	0	0.68

Table A2-1. Comparison of Tank 241-SX-113 Historical Tank Content-Based Inventory Estimates for Selected Analytes with Auger Sample Results. (2 Sheets)

Analyte	HDW model inventory estimate (kg)[a]	Analysis of auger samples[b]
PO_4	0	NR
Si	17,500	17,700
SO_4	7.55	NR
Sr	0	3.28
TOC	0	NR
Zr	0	1.36
Radionuclide (Ci)		
^{90}Sr	7,020 Ci	NR
^{137}Cs	423 Ci	NR
^{238}U	9.19 E-04 Ci (2.72 kg)	0.0048 Ci (14.2 kg)
^{239}Pu	3.57 Ci	NR

HDW = Hanford Defined Waste
NR = Not reported
[a] Agnew et al. (1997)
[b] Temer and Villarreal (1997).

A3.0 COMPONENT INVENTORY EVALUATION

The following evaluation of tank contents is performed to identify potential errors and/or missing information that would have an effect upon the HDW model component inventories.

A3.1 CONTRIBUTING WASTE TYPES

Tank 241-SX-113 is the first tank in a cascade that includes tanks 241-SX-114 and 241-SX-115. Tank 241-SX-113 was designed and constructed to be a self-boiling tank with the condensate directed back to the tank. Tank 241-SX-113 was connected to an exhauster.

Tank 241-SX-113 first received 1,843 kL (487 kgal) of Reduction and Oxidation (REDOX) process high-level waste (HLW) produced in 1958 (Anderson 1990, Brevick et al. 1994). As noted previously, REDOX process HLW produced from 1951 through 1958 is referred to as R1 waste in the HDW model. Condensate, 284 kL (75 kgal) resulting from the self-boiling nature of the HLW was removed from tank 241-SX-113 in 1958. Also in

1958, because the integrity of the tank was brought into question, 1,154 kL (305 kgal) of waste slurry (supernatant and sludge) was removed from tank 241-SX-113.

From 1958 to 1962 no wastes were added to or removed from tank 241-SX-113. In 1962, as part of a leak check test, 787 kL (208 kgal) of tank 241-SX-114 supernatant were added to tank 241-SX-113 and 681 kL (180 kgal) of such supernatant liquid immediately disappeared. The missing liquid was assumed to have leaked. At this point the tank was reported (Brevick et al. 1994) to contain 7.6 kL (2 kgal) of solids presumed to be sludge from neutralized REDOX process waste. Subsequent to the leak check test, tank 241-SX-113 remained static until 1972 when 110 kL (29 kgal) of diatomaceous earth were added to the tank.

Expected Solids in Waste

Anderson (1990):	R (REDOX process sludge), DE (Diatomaceous Earth)
Agnew et al. (1997):	R1 and DE
Hill et al. (1995):	R and DE

Predicted Current Inventory

Agnew et al. (1997)

Waste type	Waste volume
R1	7.57 kL (2 kgal)
DE	110 kL (29 kgal)

Hanlon (1996)

Waste type	Waste volume
Sludge	98 kL (26 kgal)

A3.2 EVALUATION OF TECHNICAL FLOWSHEET INFORMATION

In Table A3-1 (reproduced from Table D1-3 in Appendix D of Kupfer et al. 1997) are listed compositions for REDOX process high-level waste as stated in the HDW model (Agnew et al. 1997) for R1 waste type and as determined from REDOX process flowsheets no. 5 and 6, Kupfer et al. An average of analyte compositions specified by flowsheets no. 5 and 6 is believed to best represent the composition of the REDOX process HLW added to the tank 241-SX-113.

Table A3-1. Reduction and Oxidation Process High-Level Waste Compositions.

Component	Concentration in *M/L*			
	REDOX Process Flowsheet[a]			Predictions[b]
	No. 5	No. 6	Average[c]	R1
Al	1.29	0.95	1.12	1.13
Bi	0	4.9 E-04	2.5 E-04	0
Cr	0.17	0.13	0.15	0.113
Fe	0.0074	0.0075	0.0075	0.048
I	0	4.3 E-05	2.2 E-05	NR
K	0.0034[d]	0.0034[d]	0.0034[d]	0.021
Mn	0.0034[d]	0.0034[d]	0.0034[d]	0
Na	7.1	7.3	7.2	5.50
NO_3	4.3	3.8	4.1	2.98
Oxalate	0.0077	0.0080	0.0079	0
Si	0	0	0	0.015
SO_4	0.023	0.022	0.023	0.019
U	0.0037	0.0067	0.0022	0.0028
Issue date	8/55	10/60		

NR = Not reported
REDOX = Reduction and oxidation
[a] Adapted from Table D1-3, Appendix D of Kupfer et al. (1997)
[b] Hanford Defined Waste model (Agnew et al. 1997)
[c] Average composition of wastes produced under conditions of flowsheets no. 5 and 6, Kupfer et al. (1997)
[d] Assumed value.

REDOX process flowsheets no. 5 and 6, Kupfer et al. (1997) were published in 1955 and 1960, respectively. Except Al, Bi, and iodine, the HLW produced under conditions of flowsheet no. 6 contained the same chemical components at almost identical concentrations as that produced using flowsheet no. 5 conditions. Under flowsheet no. 6 conditions both bismuth (as $NaBiO_3$) and iodine (as HIO_4) were added during reprocessing of irradiated fuel, and slightly less aluminum nitrate nonahydrate (ANN) was used under flowsheet no. 6 conditions than under those of flowsheet no. 5. There is some uncertainty over the exact time when certain process changes were made in the REDOX plant as discussed in Appendix D of Kupfer et al. (1997). An average of the concentrations of various analytes in the REDOX process HLW streams generated using flowsheets no. 5 and 6 is believed to more correctly represent the composition of the waste introduced into tank 241-SX-113 in 1958.

The flowsheet composition data listed in Table A3-1 (derived from Appendix D of Kupfer et al. 1997) indicate that neither Mn nor K was present in the REDOX process HLW generated using flowsheets no. 5 and 6. In fact, potassium permanganate was routinely used as a REDOX process chemical throughout at least part of calendar year 1959. Therefore, the assumption in this report is that all REDOX process HLW added to tank 241-SX-113 contained 0.0034*M* $KMnO_4$; REDOX process flowsheet no. 4 lists the $KMnO_4$ concentration as 0.0034*M*.

A3.3 ASSUMPTIONS FOR RECONCILING WASTE INVENTORIES

This section presents the results of an independent assessment of the inventories of various analytes in tank 241-SX-113 waste. A set of simplified assumptions forms the basis for the independent assessment. The assumptions and observations are based upon best technical judgement pertaining to parameters that can significantly influence tank inventories. These parameters include the following:

1. Correct predictions of contributing waste types

2. Accurate predictions of model flowsheet conditions, fuel processed, and waste volumes, accurate predictions of component solubilities

3. Accurate predictions of physical parameters such as density, percent solids, void fraction (porosity), etc.

As necessary, the assumptions used can be modified to provide a basis for identifying potential errors and/or missing information that could influence either or both sample- and model-based inventories. The simplified assumptions and observations used for predicting the inventory of several analytes in tank 241-SX-113 are as follows:

1. Only the neutralized REDOX process HLW slurry introduced into tank 241-SX-113 contributed to solids formation. Waste supernatant from tank 241-SX-114 added to tank 241-SX-113 did not contribute to solids formation.

2. Radiolysis of NO_3 to NO_2 and additions of NO_2 to the waste in tank 241-SX-113 for corrosion control purposes are not accounted for in this independent assessment.

3. All Bi, Fe, Mn, Si, and U in the REDOX process HLW added to tank 241-SX-113 precipitated as water-insoluble compounds.

4. Except for those components that precipitated as solid compounds, all other analytes are assumed to have partitioned between the liquid and solid portions of the radioactive waste.

5. The concentration of analytes in the REDOX process sludge in tank 241-SX-113 is assumed to be the same as the average concentration of the same analytes in sludge in tanks 241-S-101 Kruger et al. (1996), 241-S-104 DiCenso et al. (1994), and 241-S-107 Simpson et al. (1996).

A3.4 PREDICTED INVENTORY OF ANALYTES IN TANK 241-SX-113

A3.4.1 Tank Inventory Calculated from Analysis of Auger Samples

Table A3-2 lists concentration data obtained by LANL workers from portions of the archived auger samples obtained in 1995, Temer and Villarreal (1997). The total tank inventory of each of the analytes listed was calculated as the product of the particular analyte concentration shown in column two (as g/g) and 5.61 E+04 kg, the mass of solid waste stated (Agnew et al. 1997) to be in tank 241-SX-113; and is shown in column 3.

Table A3-2. Analyte Concentrations and Analyte Total Tank Inventories of Auger Sample for Tank 241-SX-113. (2 Sheets)

Analyte	Concentration in g/g*	Sample Tank Inventory (kg)
Ag	<3.42 E-07	<0.02
Al	0.0212	1,190
B	<3.42 E-07	<0.02
Bi	8.21 E-06	0.46
Ca	0.00376	211
Cr	1.13 E-04	6.34
Fe	0.0243	1,360
K	0.00137	76.9
Mn	6.52 E-04	36.6
Na	0.00171	95.9
Ni	1.07 E-05	0.60
Pb	1.22 E-05	0.68
P	<6.84 E-05	<3.84
Si	0.315	17,700
Sr	5.84 E-05	3.28
U	2.53 E-04	14.2
Zn	1.14 E-04	6.40

Table A3-2. Analyte Concentrations and Analyte Total Tank Inventories of Auger Sample for Tank 241-SX-113. (2 Sheets)

Analyte	Concentration in g/g[a]	Sample Tank Inventory (kg)
Zr	2.43 E-05	1.36

[a] Temer and Villarreal (1997)

A3.4.2 Tank Inventory Calculated by Independent Engineering Assessment Procedure

A3.4.2.1 Contribution to Inventory from Reduction and Oxidation Process High-Level Waste. Table A3-3 lists concentration data determined for samples of sludge from tanks 241-S-101, 241-S-104, and 241-S-107. Also listed in Table A3-3 are the average concentrations (μg/g) for many of the analytes in these tanks. Convincing arguments made in TCRs for tanks 241-S-101 (Kruger et al. [1996]), 241-S-104 (DiCenso et al. [1994]), and 241-S-107 (Simpson et al. [1996]) show that the sludge in these tanks derives solely from REDOX process HLW (Hu et al. 1996). The average concentration (μg/g) of analytes determined in tanks 241-S-101, 241-S-104, and 241-S-107 is believed to also represent the composition of the REDOX process high-level sludge in tank 241-SX-113.

The sludge inventory of various analytes in tank 241-SX-113 is calculated by multiplying each of the average analyte concentrations listed in Table A3-3 by a density of 1.77 (the average density of the three comparison tanks and by 7.6 kL (2 kgal) of sludge waste, the volume of solid waste stated (Agnew et al. 1997) to be in tank 241-SX-113. Results of these computations are shown in Table A3-3. The formula used in the spreadsheet was μg/g x 3,785 L/kgal x 2 kgal x 1.77 kg/L(g/mL) x 1 g/$10^6\mu$g = kg of analyte from the sludge. For the radionuclide components, the formula used in the spreadsheet was μCi/g x 3,785 L/kgal x 2 kgal x 1.77 kg/L x 1,000 g/kg x 1 Ci/10^6 μCi = Ci of radionuclide from the sludge.

Table A3-3. R1 Sludge Concentration Estimate. (2 Sheets)

Analyte	241-S-101 segments 7U-8L[a] (μg/g)	241-S-104 (total sludge conc.)[b] (μg/g)	241-S-107 segments[c] (μg/g)	Average conc.[d] (μg/g)	HDW[e] sludge layer conc. for tank 241-SX-113	Sludge inventory for tank 241-SX-113 (kg)
Ag	9.71	<DL	<DL	9.7	NR	0.13
Al	127,000	117,000	56,400	100,000	107,000	1,340
B	63.1	26.6	49	46.2	NR	0.62
Bi	<38.8	<45.7	NR	<42.2	0	<0.57
Ca	322	247	234	268	5,020	3.59
Cl	2,050	3,200	1,860	2,370	1,040	32
Cr	2,230	2,350	1,180	1,920	1,830	25.7
F	<65.7	145	150	<120	0	<1.61
Fe	1,960	1,720	1,160	1,613	32,200	21.6
Hg	NR	<0.126	NR	<0.126	0	<0.0017
K	539	300	457	432	250	5.8
La	<19.5	<2.07	NR	<10.8	0	<0.145
Mn	2,750	1,150	83	1,330	0	17.8
Na	112,000	121,000	60,400	97,800	106,000	1,310
Ni	90.7	56	206	118	1,690	1.58
NO_2	31,100	25,900	34,300	30,433	38,200	407
NO_3	119,000	191,000	57,600	122,500	187,000	1,641
Pb	37	29.6	33	33.2	0	0.44
PO_4	1,360	<2,190	1,630	<1,730	0	23.2
P	278	93.2	391	254	NR	3.4
S	343	472	293	369	NR	4.9
Si	1,360	1,330	1,060	1,250	129	16.7
SO_4	897	2,270	1,300	1,489	569	20
Sr	456	424	378	420	0	5.6
TIC as CO_3	NR	4,140	NR	4,140	99.7	55.5
TOC	NR	1,730	NR	1,730	0	23.2
U	7,684	6,690	8,685	7,690	207	103
Zn	25.1	NR	2.4	13.8	NR	0.18

Table A3-3. R1 Sludge Concentration Estimate. (2 Sheets)

Analyte	241-S-101 segments 7U-8L[a] (μg/g)	241-S-104 (total sludge conc.)[b] (μg/g)	241-S-107 segments[c] (μg/g)	Average conc.[d] (μg/g)	HDW[e] sludge layer conc. for tank 241-SX-113	Sludge inventory for tank 241-SX-113 (kg)
Zr	36	33.6	131	66.9	0	0.90
density (g/mL)	1.77	1.64	1.90	1.77	1.76	1.77
Radionuclides[f] (μCi/g)						
^{90}Sr	NR	301	276	288	529	3,860 Ci
^{137}Cs	98	60.5	74	77.6	31.9	1,040 Ci

NR = Not reported
HDW = Hanford Defined Waste
[a] Kruger et al. (1996)
[b] DiCenso et al. (1994)
[c] Statistically determined median R1 sludge concentrations for tank 241-S-107 contained in the attachment to Simpson et al. (1996)
[d] Average of analyte concentrations for tank 241-S-101, 241-S-104, and 241-S-107
[e] Agnew et al. (1997) for Tank 241-SX-113 (R1 Waste portion only)
[f] Radionulcides decayed to January 1, 1994.

A3.4.2.2 Contribution to Inventory from Diatomaceous Earth. In 1972 three truck loads, approximately (4.08 E+04 kg) of diatomaceous earth were added to tank 241-SX-113 (Buckingham and Metz 1974).

The nominal composition of diatomaceous earth is as follows (all wt%):

Al_2O_3 - 1.1 Al - 0.58
CaO - 0.9 Ca - 0.64
Fe_2O_3 - 2.0 Fe - 1.4
SiO_2 - 92.3 Si - 43.1
MgO - 0.4 (Mg not reported in best-basis)

Given this composition and assuming that all the components of the diatomaceous earth remained in the tank, 45 tons (4.08 E+04 kg) of diatomaceous earth contributed the following listed quantities of material (stated on an elemental basis) to the inventory of waste in tank 241-SX-113:

SiO_2 - 92.3 Si - 43.1
MgO - 0.4 (Mg not reported in best-basis)

Given this composition and assuming that all the components of the diatomaceous earth remained in the tank, 45 tons (4.08 E+04 kg) of diatomaceous earth contributed the following listed quantities of material (stated on an elemental basis) to the inventory of waste in tank 241-SX-113:

Sample calculation for Al: 0.0058 x 40,800 kg = 237 kg

Element	kg
Al	237
Si	17,600
Ca	261
Fe	571

The inventory from diatomaceous earth for these four analytes is added to those for the sludge and are shown in Table A3-4.

The exact long-term chemical behavior of the diatomaceous earth added to tank 241-SX-113 is not known. Buckingham and Metz (1974) noted that SiO_2 in diatomaceous earth can undergo one of two principal reactions:

$$NaAlO_2 + SiO_2 + 0.7\ H_20 = NaAlSiO_4 \cdot 0.7\ H_20$$

$$2\ NaOH + SiO_2 = Na_2SiO_3 + H_2O$$

For charge balance purposes, Agnew et al. (1996) in the HDW model assumed that the added SiO_2 reacted to form Na_2SiO_3. The same assumption, made here in the independent engineering assessment, leads to the presence of 28 MT of sodium deriving from the stoichiometric amount of NaOH required to react with 17.5 MT of silicon. There is no evidence that the silicon in this tank reacted in either of the above ways to any significant degree. The measured sodium in the tank does not support such reactions of having occurred to any significant degree. The purpose of adding the diatomaceous earth was to bind the sludge and having added additional sodium would have been counter productive as it would have solubilized the silicon.

Total contributions to the tank 241-SX-113 inventory from both REDOX process HLW and diatomaceous earth are listed in Table A3-4.

Inventory Comparisons

The HDW, sample-based and the engineering assessment inventories are compared in Table A3-4 and in the observations that follow the table.

Table A3-4. Comparison of Tank 241-SX-113 Historical Tank Content-Based Inventory Estimates for Selected Analytes with Engineering Assessment Estimates.[a]

Nonradioactive analyte	HDW model inventory estimate (kg)[b]	Engineering assessment (kg)[d]	Analysis of auger samples[c]
Al	1,660	1,580[d]	1,190
Bi	0.00	<0.57	0.46
Ca	419	265[d]	211
Cl	13.8	32.0	NR
TIC as CO_3	99.7	55.5	NR
Cr	24.3	25.7	6.34
Fe	979	593[d]	1,360
Hg	0	<0.0017	NR
K	3.32	5.8	76.9
La	0	<0.145	NR
Mn	0.00	17.8	36.6
Na	28,300	1,310	95.9
Ni	22.5	1.58	0.60
NO_2	507	407	NR
NO_3	2,480	1,641	NR
Pb	0.00	0.44	0.68
PO_4	0.00	<23.2	NR
Si	17,500	17,600[d]	17,700
SO_4	7.55	20.0	NR
Sr	0.00	5.6	3.28
TOC	0.00	23.2	NR
Zr	0.00	0.87	1.36
Radionuclide[e] (Ci)			
^{90}Sr	7,020 Ci	3,860 Ci	NR
^{137}Cs	423 Ci	1,040 Ci	NR

HDW = Hanford Defined Waste
NR = Not reported
[a] Methodology for engineering assessment
[b] Agnew et al. (1997)
[c] Temer and Villarreal (1997)
[d] Includes inventory from Diatomaceous Earth.
[e] Radionuclides decayed to January 1, 1994.

Aluminum. Three values are listed in Table A3-4 for the aluminum content of tank 241-SX-113. The HDW model predicts this tank to contain 1,660 kg of aluminum. Calculations based upon analysis of auger samples indicate tank 241-SX-113 to contain 1,190 kg of aluminum. Finally, an independent engineering analysis based upon the composition and amount of diatomaceous earth and on the calculated composition (from data for tanks 241-S-101, 241-S-104, and 241-S-107) of the REDOX process sludge leads to a value of 1,580 kg of aluminum. Of this amount, 237 kg of aluminum arose from diatomaceous earth added to the tank in 1972. The 1,580 kg from the engineering assessment was selected as the best-basis inventory estimate.

Bismuth. The HDW model predicts that waste in tank 241-SX-113 contains no bismuth. This prediction is not correct since at least some of the REDOX process HLW contained bismuth, albeit at very low concentration. In point of fact, the HDW model simply did not include bismuth in REDOX process waste as one of its parameters. Based on analysis of auger samples for tank 241-SX-113, a bismuth inventory of 0.46 kg is predicted. This value is in reasonable agreement with the inventory of <0.57 kg predicted by an independent engineering analysis based upon the average composition of REDOX process sludge in tanks 241-S-101, 241-S-104, and 241-S-107. The engineering assessment value of <0.57 was selected as the best-basis inventory estimate.

Calcium. Calcium entered tank 241-SX-113 both as a constituent of diatomaceous earth added to the tank in 1972 and as an impurity in the commercial-grade NaOH used to neutralize the acidic REDOX process HLW added to the tank in 1958. The diatomaceous earth added to the tank is estimated to have contributed 261 kg of calcium. The HDW model predicts tank 241-SX-113 to contain 419 kg of calcium while direct analyses of auger samples from the tank indicate a tank calcium inventory of 211 kg. The engineering assessment value of 265 kg was selected as the best-basis calcium inventory estimate.

Carbonate. Carbonate in the waste in tank 241-SX-113 presumably formed by sorption of CO_2 from the air by NaOH in the tank. The HDW model predicts that tank 241-SX-113 contains 99.7 kg of carbonate. The engineering assessment predicts 55.5 kg of carbonate. This is accepted as the best-basis value.

Chloride. Auger samples from tank 241-SX-113 were not analyzed for chloride content. The HDW model predicts tank 241-SX-113 to contain 13.0 kg of chloride while an independent engineering assessment based upon the assumption that the REDOX process HLW sludge in the tank has the same composition as the average composition of the sludges in tanks 241-S-101, 241-S-104, and 241-S-107 leads to a calculated 32 kg of chloride. For best-basis inventory purposes the engineering assessment of 32 kg chloride is chosen.

Chromium. Throughout its operation, the REDOX process used sodium dichromate to oxidize plutonium to the extractable +6 state. When the REDOX process waste was made alkaline for interim storage most of the chromium remained as soluble Cr(VI) but some of the chromium was reduced to Cr(III) which precipitated as a hydrated oxide.

The HDW model (Rev. 4) predicts the solid waste in tank 241-SX-113 to contain 24.3 kg of chromium, a value in close agreement with the 25.7 kg predicted by an independent engineering assessment based upon the average composition of REDOX process sludges in tanks 241-S-101, 241-S-104, and 241-S-107. Direct analysis of auger samples from tank 241-SX-113 indicates that the tank only contains 6.34 kg of chromium. There is the possibility that the auger sample was not completely representative of all the waste in tank 241-SX-113. For this reason, the engineering assessment of 25.7 kg was selected as the best-basis estimate of the chromium content of tank 241-SX-113.

Total Hydroxide. Once the best-basis inventories were determined, the hydroxide inventory was calculated by performing a charge balance with the valences of other analytes. In some cases, this approach requires that other analyte (e.g., sodium or nitrate) inventories be adjusted to achieve the charge balance. During such adjustments, the number of significant figures is not increased. This charge balance approach is consistent with that used by Agnew et al. (1997).

Iron. Three predictions of the iron content of tank 241-SX-113 are available (Table A3-4). The HDW model predicts tank 241-SX-113 to contain 979 kg of iron. The HDW model prediction is in reasonable agreement with the value 1,360 kg calculated from analysis of auger samples taken from tank 241-SX-113. An independent engineering analysis based upon the assumption that the composition of REDOX process sludge in tank 241-SX-113 is the same as the average of the compositions of the same type of sludge in tanks 241-S-101, 241-S-104, and 241-S-107 leads to a value of only 593 kg of iron in the tank. This value also includes the iron contribution from diatomaceous earth added to the tank. The sample based value of 1,360 was selected as the best-basis iron inventory in tank 241-SX-113.

Manganese. The HDW model (Rev. 4) does not predict tank 241-SX-113 to contain any manganese. This result is the expected one since the composition of REDOX process HLW (R1) used in model calculations did not specify that manganese was present. This latter composition is in error because REDOX process HLW generated through the fall of 1959 is known to have contained at least some manganese. From direct analyses of auger samples of the waste in tank 241-SX-113 the tank is estimated to contain 36.6 kg of manganese. An independent engineering assessment based on the average of the composition of REDOX process sludge in tanks 241-S-101, 241-S-104, and 241-S-107 leads to a value of 17.8 kg of manganese in tank 241-SX-113. Finally, a separate calculation based upon the volume of REDOX process waste added to tank 241-SX-113 at an assumed manganese concentration of 0.0034*M* leads to a value of 50.9 kg. For best-basis inventory purposes, the sample-based value of 36.6 kg was selected.

Nickel. The HDW model predicts tank 241-SX-113 to contain as much as 22.5 kg of nickel. The other two prediction bases, i.e., assessment based upon analysis of auger samples and calculations based upon an assumed average composition of REDOX process sludge (tanks 241-S-101, 241-S-104, and 241-S-107), account for very much less nickel, 0.60 and 1.58 kg, respectively. Nickel in REDOX process sludge is believed to have arisen from

two sources, namely corrosion of stainless steel equipment and as a minor component in Al-clad uranium metal fuel. It is also believed that the HDW model seriously overestimates the amount of stainless steel corrosion which occurred in REDOX process operation. The engineering assessment of 1.58 kg was selected as the best-basis inventory of nickel in tank 241-SX-113.

Nitrate. The HDW model predicts tank 241-SX-113 to contain 2,480 kg of nitrate. The independent engineering assessment based upon the assumption that the REDOX sludge in tank 241-SX-113 has the same composition as the average of the sludges in tanks 241-S-101, 241-S-104, and 241-S-107 leads to a predicted nitrate inventory of 1,641 kg. Note that the auger samples taken from tank 241-SX-113 were not analyzed for their nitrate content. The best-basis estimate of the nitrate inventory in tank 241-SX-113 is 1,641 kg, the engineering assessment value.

Nitrite. The HDW model predicts tank 241-SX-113 to contain 507 kg of nitrite. The independent engineering assessment based upon the assumption that the REDOX process sludge in tank 241-SX-113 has the same composition as the average of the REDOX process sludge in tanks 241-S-101, 241-S-104, and 241-S-107 leads to a predicted nitrite inventory of 407 kg, a value in reasonable agreement with the HDW model prediction. Note that the auger samples taken from tank 241-SX-113 were not analyzed for their content of nitrite. The best-basis inventory estimate of nitrite in tank 241-SX-113 is 407 kg, the engineering assessment value.

Potassium. Potassium was introduced into tank 241-SX-113 by two mechanisms:

1. Known $KMnO_4$ added to REDOX process feedstock

2. As an impurity in the commercial-grade NaOH used to neutralize acidic REDOX process HLW.

The HDW model did not take into account any $KMnO_4$ present in waste added to the tank. Thus, the HDW estimate of 3.32 kg potassium presumably reflects the impurity level in the NaOH added to the REDOX process waste. The two other predictions (Table A3-4) of the potassium inventory of tank 241-SX-113 are both higher than the HDW model estimate, namely 5.8 and 76.9 kg. The sample-based estimate of 76.9 kg was picked as the best-basis to be conservative, since that is the amount measured in the sample.

Silicon. All the three different prediction bases (Table A3-4) state that tank 241-SX-113 contains about 17,600 kg of silicon. That all these assessments should lead to the same silicon inventory is not surprising since all are based upon the addition of 45 tons of diatomaceous earth to the tank. The fact that direct analysis of the auger samples also provides a silicon inventory of about 17,700 kg is good evidence that at least the top material in the tank was satisfactorily sampled.

Sodium. Inspection of the sodium data in Table A3-4 quickly reveals a wide disparity is the three predictions of the inventory of sodium in tank 241-SX-113. Analysis of auger samples from the tank indicate an impossibly low value of 95.9 kg. Conversely, the HDW model estimate of 28,300 kg sodium is highly questionable since Agnew et al. (1997) assumed this quantity of sodium was required for charge balance purposes assuming all the silicon was present as the doubly negative charged SiO_3 species. The best-basis inventory value of 1,310 kg sodium derives from the independent engineering assessment which assumes that the composition of REDOX process sludge in tank 241-SX-113 is the same as the average composition of REDOX process sludge in tanks 241-S-101, 241-S-104, and 241-S-107.

Sulfate. The HDW model assumes that sulfate ion, derived from ferrous sulfamate used in REDOX process operations, was largely soluble in neutralized REDOX process HLW. On this very reasonable basis, the HDW model predicts tank 241-SX-113 to only contain 7.55 kg of sulfate. An independent engineering analysis based upon the assumption that the composition of REDOX process sludge in tank 241-SX-113 is the same as the average composition of REDOX process sludge in tanks 241-S-101, 241-S-104, and 241-S-107 leads to a calculated sulfate inventory of 20 kg. The engineering assessment value of 20 kg, was selected as the best-basis inventory value.

Uranium. The HDW model predicts tank 241-SX-113 to only contain 2.75 kg (9.19 E-04 Ci) of uranium (as ^{238}U). Conversely, an independent engineering analysis based upon the average composition of the REDOX process sludge in tanks 241-S-101, 241-S-104, and 241-S-107 predicts the tank to contain 103 kg of uranium. Uranium in auger samples resulted in a predicted inventory of 14.2 kg. The engineering assessment value of 103 kg, was selected as the best-basis uranium inventory estimate for tank 241-SX-113.

A4.0 DEFINE THE BEST-BASIS AND ESTABLISH COMPONENT INVENTORIES

An effort is underway to provide waste inventory estimates that will serve as standard characterization source terms for the various waste management activities (Hodgson and LeClair 1996). As part of this effort, an evaluation of chemical information for tank 241-A-102 was performed, and a best basis inventory was established. This work, detailed in the following sections, follows the methodology that was established by the standard inventory task. The following information was utilized as part of this evaluation:

- Inventory estimates generated by HDW model (Agnew et al. 1997)
- Inventory estimates generated by a tank-specific assessment process utilizing chemical process flowsheets and a detailed historical tank waste transaction data base.
- A combination of inventory estimates provided by a partial chemical analysis of analytes in auger samples data from tank 241-SX-113.

The results from this evaluation support using a predicted inventory based primarily on results from the tank-specific assessment process supplemented, in a few instances, by predictions of the HDW model and analytical data for the following reasons:

- The waste in tank 241-SX-113 has not been adequately sampled, it is not possible to predict a high quality inventory based on available analytical results.
- Both the HDW model and the tank-specific assessment approaches correctly postulate that solids in tank 241-SX-113 arose from addition of diatomaceous earth and REDOX process HLW to the tank.
- Published and well-established REDOX process chemical flowsheets were used in tank-specific inventory calculations. Conversely, chemical flowsheets used in developing the HDW model for tank 241-SX-113 differed significantly from the published versions.
- Available analytical data, in many instances, support analyte inventory predictions based on the HDW model and/or the independent engineering analysis.

Best-basis tank inventory values are derived for 46 key radionuclides (as defined in Section 3.1 of Kupfer et al. 1997), all decayed to a common report date of January 1, 1994. Often, waste sample analyses have only reported ^{90}Sr, ^{137}Cs, $^{239/240}$Pu, and total uranium (or total beta and total alpha), while other key radionuclides such as ^{60}Co, ^{99}Tc, ^{129}I, ^{154}Eu, ^{155}Eu, and ^{241}Am, etc., have been infrequently reported. For this reason it has been necessary to derive most of the 46 key radionuclides by computer models. These models estimate radionuclide activity in batches of reactor fuel, account for the split of radionuclides to

various separations plant waste streams, and track their movement with tank waste transactions. (These computer models are described in Kupfer et al. 1997, Section 6.1 and in Watrous and Wootan 1997.) Model generated values for radionuclides in any of 177 tanks are reported in the HDW Rev. 4 model results (Agnew et al. 1997). The best-basis value for any one analyte may be either a model result or a sample or engineering assessment-based result if available. (No attempt has been made to ratio or normalize model results for all 46 radionuclides when values for measured radionuclides disagree with the model.) For a discussion of typical error between model derived values and sample derived values, see Kupfer et al. 1997, Section 6.1.10.

The inventory values reported in Tables A4-1 and A4-2 are subject to change. Refer to the Tank Characterization Database (TCD) for the most current inventory values.

Table A4-1. Best-Basis Inventory Estimates for Nonradioactive Components in Tank 241-SX-113 (Effective January 31, 1997). (2 Sheets)

Analyte	Total inventory (kg)	Basis (S, M, E, or C)[1]	Comment
Al	1,580	E	
Bi	<0.57	E	
Ca	265	E	
Cl	32.0	E	
TIC as CO_3	55.5	E	
Cr	25.7	E	
F	<1.61	E	Not determined in S
Fe	1,360	S	
Hg	<0.0017	E	
K	76.9	S	E reported 5.8
La	<0.145	E	
Mn	36.6	S	E reported 17.8
Na	1,310	E	
Ni	1.58	E	S reported 0.60
NO_2	407	E	
NO_3	1,640	E	
OH_{TOTAL}	3,420*	C	*Assumed only 2 kgal of DE for Si (1,220 kg) interacted with sludge for charge balance purposes
Pb	0.68	S	E reported 0.45
PO_4	<23.2	E	Not determined in S or M
Si	17,700	S	Known amount of diatomaceous earth added
SO_4	20	E	
Sr	5.6	E	S reported 3.28
TOC	23.2	E	Not determined in S
U_{TOTAL}	103	E	

Table A4-1. Best-Basis Inventory Estimates for Nonradioactive Components in Tank 241-SX-113 (Effective January 31, 1997). (2 Sheets)

Analyte	Total inventory (kg)	Basis (S, M, E, or C)[1]	Comment
Zr	1.36	S	E reported 0.90

[1]S = Sample-based
M = Hanford Defined Waste model-based, Agnew et al. (1997)
E = Engineering assessment-based
C = Calculated by charge balance; includes oxides as hydroxides, not including CO_3, NO_2, NO_3, PO_4, SO_4, and SiO_3.

Table A4-2. Best-Basis Inventory Estimates for Radioactive Components in Tank 241-SX-113 Decayed to January 1, 1994 (Effective January 31, 1997). (2 Sheets)

Analyte	Total inventory (Ci)	Basis (S, M, or E)[1]	Comment
^{3}H	0.221	M	
^{14}C	0.0171	M	
^{59}Ni	0.112	M	
^{60}Co	0.00675	M	
^{63}Ni	10.5	M	
^{79}Se	0.00363	M	
^{90}Sr	3,860	E	
^{90}Y	1,040	E	From ^{90}Sr
^{93}Zr	0.0171	M	
^{93m}Nb	0.0140	M	
^{99}Tc	0.120	M	
^{106}Ru	1.89 E-08	M	
^{113m}Cd	0.0582	M	
^{125}Sb	0.00992	M	
^{126}Sn	0.00558	M	
^{129}I	2.30 E-04	M	
^{134}Cs	2.05 E-04	M	
^{137}Cs	1,040	E	
^{137m}Ba	984	E	From ^{137}Cs
^{151}Sm	13.0	M	
^{152}Eu	0.0592	M	
^{154}Eu	0.163	M	
^{155}Eu	2.50	M	
^{226}Ra	8.17 E-06	M	
^{227}Ac	3.60 E-05	M	
^{228}Ra	7.00 E-11	M	
^{229}Th	1.34 E-08	M	
^{231}Pa	5.43 E-06	M	
^{232}Th	4.47 E-12	M	
^{232}U	3.96 E-08	M	

Table A4-2. Best-Basis Inventory Estimates for Radioactive Components in Tank 241-SX-113 Decayed to January 1, 1994 (Effective January 31, 1997). (2 Sheets)

Analyte	Total inventory (Ci)	Basis (S, M, or E)[1]	Comment
^{233}U	1.51 E-09	M	
^{234}U	9.01 E-04	M	
^{235}U	3.88 E-05	M	
^{236}U	1.42 E-05	M	
^{237}Np	7.77 E-04	M	
^{238}Pu	0.0500	M	
^{238}U	9.19 E-04	M	
^{239}Pu	3.57	M	
^{240}Pu	0.511	M	
^{241}Am	0.0612	M	
^{241}Pu	3.00	M	
^{242}Cm	0.00122	M	
^{242}Pu	1.38 E-05	M	
^{243}Am	5.72 E-07	M	
^{243}Cm	2.79 E-05	M	
^{244}Cm	2.04 E-05	M	

[1]S = Sample-based
M = Hanford Defined Waste model-based, Agnew et al. (1997)
E = Engineering assessment-based

A5.0 APPENDIX A REFERENCES

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