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Preliminary Tank Characterization Report for Single-Shell Tank 241-SX-112: Best-Basis Inventory

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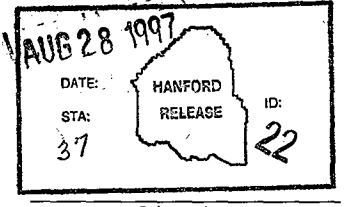
Abstract: An effort is underway to provide waste inventory estimates that will serve as standard characterization source terms for the various waste management activities. As part of this effort, an evaluation of available information for single-shell tank 241-SX-112 was performed, and a best-basis inventory was established. This work follows the methodology that was established by the standard inventory task.



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PRELIMINARY TANK CHARACTERIZATION REPORT FOR SINGLE-SHELL TANK 241-SX-112: BEST-BASIS INVENTORY

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PRELIMINARY TANK CHARACTERIZATION REPORT FOR SINGLE-SHELL TANK 241-SX-112: BEST-BASIS INVENTORY

This document is a preliminary Tank Characterization Report (TCR). It only contains the current best-basis inventory (Appendix D) for single-shell tank 241-SX-112. No TCRs have been previously issued for this tank, and current core sample analyses are not available. The best-basis inventory, therefore, is based on an engineering assessment of waste type, process flowsheet data, early sample data, and/or other available information.

The *Standard Inventories of Chemicals and Radionuclides in Hanford Site Tank Wastes* (Kupfer et al. 1997) describes standard methodology used to derive the tank-by-tank best-basis inventories. This preliminary TCR will be updated using this same methodology when additional data on tank contents become available.

REFERENCE

Kupfer, M. J., A. L. Boldt, B. A. Higley, K. M. Hodgson, L. W. Shelton, B. C. Simpson, and R. A. Watrous (LMHC), S. L. Lambert, and D. E. Place (SESC), R. M. Orme (NHC), G. L. Borsheim (Borsheim Associates), N. G. Colton (PNNL), M. D. LeClair (SAIC), R. T. Winward (Meier Associates), and W. W. Schulz (W^2S Corporation), 1997, *Standard Inventories of Chemicals and Radionuclides in Hanford Site Tank Wastes*, HNF-SD-WM-TI-740, Rev. 0, Lockheed Martin Hanford Corporation, Richland, Washington.

APPENDIX D

EVALUATION TO ESTABLISH BEST-BASIS INVENTORY FOR SINGLE-SHELL TANK 241-SX-112

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APPENDIX D

EVALUATION TO ESTABLISH BEST-BASIS INVENTORY FOR SINGLE-SHELL TANK 241-SX-112

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-112 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 sections establish a best-basis inventory estimate for chemical and radionuclide components in tank 241-SX-112. A complete list of data sources and inventory evaluations is provided at the end of this section.

D1.0 CHEMICAL INFORMATION SOURCES

The waste in tank 241-SX-112 has not been core sampled and analyzed. A Tank Characterization Report (TCR) for tank 241-SX-112 has not been prepared. The Hanford Defined Waste (HDW) model report (Agnew et al. 1997) provides tank content estimates in terms of component concentrations and inventories.

Tank 241-SX-112 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.

D2.0 COMPARISON OF COMPONENT INVENTORY VALUES

Hanlon (1996) states that tank 241-SX-112 contains 348 kL (92 kgal) of solids and no drainable interstitial liquid or pumpable liquid. Agnew et al. (1997) concur with Hanlon's estimate. According to the HDW model, the solid waste in tank 241-SX-112 contains 30.2 wt% water and has a density of 1.74 g/cc. As described more fully later, Agnew et al. hypothesize that the solids in tank 241-SX-112 derive from both Reduction and Oxidation (REDOX) process high-level waste (HLW) and salt cake produced from concentrated REDOX process supernatant liquid added to the tank. An independent analysis of historical waste transaction data, conducted in connection with preparation of this Section, indicates that all the solid waste in tank 241-SX-112 derives only from REDOX process HLW. As

explained in detail later, the completeness and quality of the historical waste transaction data are insufficient to allow an unequivocal determination of the origin of the solid wastes now in tank 241-SX-112.

The HDW model predictions of the inventory of the various analytes in tank 241-SX-112 are listed in Table D2-1. (The chemical species are reported without charge designation per the best-basis inventory convention.)

Table D2-1. Estimated Analyte Inventories for tank 241-SX-112. (2 Sheets)

Analyte	HDW model[a] (kg)
Nonradioactive	
Al	60,600
Bi	0.125
Ca	3,660
Cl	899
CO_3	5,510
Cr	4,590
F	0.586
Fe	23,700
Hg	0.0188
K	226
Mn	0.239
Na	67,000
Ni	1,230
NO_2	25,500
NO_3	82,900
OH	156,000
Pb	3.09
PO_4	3.68
Si	1,620
SO_4	666
TOC	7.8
Zr	0.00545

Table D2-1. Estimated Analyte Inventories for tank 241-SX-112. (2 Sheets)

Analyte	HDW model[a] (kg)
Radioactive[b]	
^{239}Pu	223 Ci
^{238}U	0.127 Ci (374 kg)

HDW = Hanford Defined Waste
NR = Not reported
[a] Agnew et al. (1997)
[b] Decayed to January 1, 1994.

D3.0 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.

D3.1 CONTRIBUTING WASTE TYPES

Tank 241-SX-112 is the third (million gallon) tank in a cascade that includes tanks 241-SX-110 and 241-SX-111. Tank 241-SX-112 was constructed in the early 1950's and was designed to be a self-boiling tank with the condensate directed back to the tank. Tank 241-SX-112 was connected to an exhauster.

High-level REDOX process waste (R) was first added to tank 241-SX-112 in 1956. In 1957, 1960, 1961, and 1966, tank 241-SX-112 received additional REDOX process HLW (Brevick et al. 1994, Anderson 1990). In 1965 tank 241-SX-112 also received a one-time addition of concentrated REDOX process HLW supernatant liquid. All the high-level REDOX process waste additions are known or are believed to have contributed to the solid waste (348 kL [92 kgal]) now stored in tank 241-SX-112. Beyond such waste additions, there were many liquid transfers into and out of tank 241-SX-112 including water, condensate from self-boiling tanks including tank 241-SX-112 and supernatant liquid from other SX Tank Farm tanks. These latter liquid additions are thought to have significantly reduced the volume of REDOX process salt cake in tank 241-SX-112 as discussed in more detail later in this section.

Table D3-1 provides a summary of the transactions which may have contributed to the type and volume of wastes now in tank 241-SX-112. These values are taken from the more detailed records of waste transactions compiled by Anderson (1990) and Brevick et al. (1994).

Table D3-1. Summary of Contributing Waste Types for Tank 241-SX-112[a,b]

Historical waste transaction	Waste type	
	R	RSLTCK
Volume waste added, kL (kgal)		
1956	3,755 (992)	
1957	34.1 (9)	
1960	1,400 (370)	
1961	1,654 (437)	
1965		2,104 (556)
1966	2,419 (639)	
Volume solids, kL (kgal)		
1956	165 (43.7)[c]	
1957	1.51 (0.4)[c]	
1960	61.7 (16.3)[c,d]	
1961	72.7 (19.2)[c,d]	
1965		87.1 (23)[e]
1966	106 (28.1)[c,d]	

R = Reduction and Oxidation (REDOX) Process high-level waste
RSLTCK = REDOX Process salt cake waste
[a] From Agnew et al. (1997)
[b] From Anderson (1990)
[c] 4.4 vol% of added volume of REDOX process high-level waste
[d] Agnew et al. (1997) assumed 2.3 vol% solids from added REDOX process high-level waste
[e] Solids = 4.14 vol% of total waste slurry.

Careful review and analysis of the data summarized in Table D3-1 and other data of Anderson (1990) and Brevick et al. (1994) leads to two possible ways of accounting for the solid waste presently residing in tank 241-SX-112. One of these is due to Agnew et al. (1997) published in the HDW model (Rev. 4) report. Agnew et al. accept that the volume (measured) of waste now in tank 241-SX-112 is 348 kL (92 kgal). They partition the amount of solid waste into three types:

- 167 kL (44 kgal) of solids (4.4 vol% of 3,789 kL [1,001 kgal]) of R1 type waste
- 94.6 kL (25 kgal) of solids (2.3 vol% of 5,473 [1,446 kgal]) of R2 type waste

- 87.1 kL (23 kgal) of REDOX process salt cake

An alternative way of accounting for the solid waste now in tank 241-SX-112 involves the following analysis and evaluation:

- 166.7 kL (44.1 kgal) of solids (4.4 vol% of 3,789 k L [1,001 kgal]) of REDOX process HLW produced under the conditions of REDOX process Flowsheet 5.
- 134.4 kL (35.5 kgal) of solids (4.4 vol% of 3,054 kL [807 kgal]) of REDOX process HLW produced under the conditions of REDOX process Flowsheet 6.
- 106 kL (28.1 kgal) of solids (4.4 vol% of 2,419 kL [639 kgal]) of REDOX process HLW produced under the conditions of REDOX process Flowsheet 9.
- Negligible volume of REDOX process salt cake.

The second alternative accounts for 407 kL (107.7 kgal) of solid waste in tank 241-SX-112 versus the measured 348 kL (92) kgal. The difference of 59 kL (15.6 kgal) is believed to be outside the expected volume measurement error. Some compaction of the hydrous solids likely occurred over time. The volume difference may also be accounted for, in part, by a slight overstatement, i.e., 4.4 vol% versus 4.2 vol%, in the volume of solids precipitated from the neutralized REDOX process HLW. The 4.4 vol% value is retained in this section to be consistent with Agnew et al. (1997) and to be consistent with other sections of this report dealing with tanks containing REDOX process HLW.

In agreement with Agnew et al. (1997) it is thought that 166.7 kL (44.1 kgal) of solids resulted from REDOX process HLW generated in 1956 and 1957. This volume of solids is equivalent to 4.4 vol% of the total volume of waste added to the tank in this time frame period. Further, it also is thought 4.4 vol% (240 kL = 63.6 kgal) of solid waste resulted from the addition of REDOX process HLW added to tank 241-SX-112 in the period 1960 through 1966. The composition of REDOX process HLW produced in these latter years was almost identical to that produced in 1956, at least for iron and other constituents which precipitated when the waste was made alkaline. There is no evidence to support the Agnew et al. contention that the volume of solids precipitated from REDOX process HLW produced in the years 1960 through 1966 was substantially less, 2.3 vol% versus 4.4 vol%, than the volume of solids precipitated from REDOX process HLW generated in 1956.

In 1965, 2,104 kL (556 kgal) of evaporated REDOX process HLW supernatant liquid were added to tank 241-SX-112. This volume of waste contained, according to Agnew et al. (1997), about 4.1 vol% of solids (87.1 kL = 23 kgal). In applying the HDW model to tank 241-SX-112, Agnew et al. assumed that the REDOX process salt cake solids added in 1965 are still present in the tank. This assumption could be in error since it ignores the large amounts of water and dilute supernatant liquids added to the tank in the years subsequent to the addition of the evaporated HLW supernatant.

For example, from 1966 to 1969, 1.325 kL (350 kgal) of water were added to the tank. In the same time frame, 2,419 kL (639 kgal) of REDOX process HLW slurry were added to tank 241-SX-112. Previous laboratory experience (Schulz 1980) has shown that actual REDOX process salt cake is readily soluble in water. Thus, for the purposes of this independent engineering assessment, it is judged that all the salt cake solids present in the tank in 1965 were dissolved by the time the last liquid was pumped from the tank in 1969. This judgement is made even though it is recognized that much of the liquid added to tank 241-SX-112 boiled off and that water added to the tank served only to maintain a constant liquid level. The liquids added to the tank were not saturated in salts and, therefore, could and, it is thought, did dissolve all the soluble salt cake solids.

In summary, whereas Agnew et al. (1997) in the HDW model report (Rev. 4) conclude that salt cake solids are present in tank 241-SX-112 the independent engineering assessment described in this section concludes that such solids are not present. Obviously, both conclusions cannot be correct. The available historical waste transaction history (Anderson 1990, Brevick et al. 1994) are not sufficient to decide between the two conclusions. Final resolution of the issues will be possible only when (and if) the waste solids in tank 241-SX-112 are sampled and analyzed.

Expected Solids in Waste

Anderson (1990): R
Agnew et al. (1997): R1, R2, RSLTCK
This Evaluation: R

Predicted Current Inventory

Agnew et al. (1997)

Waste Type	Waste Volume 348 kL (92 kgal)
R1	167 kL (44 kgal)
R2	94.6 kL (25 kgal)
RSLTCK	87.1 kL (23 kgal)

Hanlon (1996)

Waste Type	Waste Volume 348 kL (92 kgal)
Sludge	

This Evaluation

Waste Type	Waste Volume 407 kL (107.6 kgal)
R (1956-57)	166.7 kL (44.1 kgal)
R (1960-61)	134.4 kL (35.5 kgal)
R (1966)	106 kL (28.1 kgal)

D3.2 EVALUATION OF TECHNICAL FLOWSHEET INFORMATION

In Table D3-2 (reproduced from information in Kupfer et al. 1997) are listed compositions for REDOX process HLW produced according to Flowsheets 5, 6, and 9. Note that the compositions of REDOX process R1 and R2 waste (Agnew et al. 1997 designations) are listed in Table D2-1 of the best-basis inventory writeup for tank 241-SX-108 (Kupfer and Schulz 1997).

Table D3-2. Composition of Reduction and Oxidation Process High-Level Waste.[a] (2 Sheets)

Composition *M*	REDOX process high-level waste		
Analyte	Flowsheet 5	Flowsheet 6	Flowsheet 9
Al	1.29	0.95	1.2
Bi	0	4.9 E-05	7.6 E-05
Cr	0.17	0.13	0.19
Fe	0.0074	0.0075	0.016
I	0	4.3 E-05	6.8 E-05
K	0.0034	0.0034[b]	0
Mn	0.0034	0.0034[b]	0
Na	7.1	7.3	6.7
NO_3	4.3	3.8	4.9
Oxalate	0.0077	0.0080	0.012
SO_4	0.023	0.022	0.031
U	0.0037[c]	6.6 E-04[c]	8.1 E-04[c]
Issue Date	8/55	10/60	9/66

REDOX = Reduction and oxidation

[a] Adapted from tables in Kupfer et al. (1997)

[b] Not shown on published flowsheet, Kupfer et al. (1997) but $KMnO_4$ usage in REDOX plant is known to have continued until the fall of 1959

[c] Table D2-1, Kupfer et al. (1997).

The composition listed in Table D3-2 for REDOX process Flowsheet 6 HLW, Kupfer et al. (1997) specifies that the waste contained 0.0034*M* $KMnO_4$. The published version of Flowsheet 6 does not include any mention of $KMnO_4$; information presented elsewhere in Kupfer et al. 1997 indicates that $KMnO_4$ was used in the REDOX process through most of 1959. Also, note as mentioned previously, that REDOX process HLW generated under

either the conditions of Flowsheets 5, 6, and 9, Kupfer et al. (1997) contained almost identical concentrations of precipitable metals, e.g., Fe, Mn, Bi, and U.

D3.3 PREDICTED WASTE INVENTORIES

This section presents results of an independent assessment of the inventories of the various analytes in tank 241-SX-112 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: (a) correct predictions of contributing waste types, (b) accurate predictions of model flowsheet conditions, fuel processed, and waste volumes, (c) accurate predictions of component solubilities, and (d) accurate predictions of physical parameters such as density, percent solids, void fraction (porosity), etc. Of course, 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-112 are as follows:

1. Only the neutralized REDOX process HLW introduced into tank 241-SX-112 contributed to solids formation. Condensates, water, and waste supernatants, either concentrated or dilute, from other SX Tank Farm tanks or evaporators added to tank 241-SX-112 did not contribute any solid waste to the inventory presently in tank 241-SX-112.

2. For all REDOX process HLW added to tank 241-SX-112 the volume of precipitated solids was 4.4 vol% of the total volume of waste slurry.

3. All Bi, Fe, Mn, Si, and U in the REDOX process HLW added to tank 241-SX-112 precipitated as solid compounds.

4. Aside from Bi, Fe, Mn, Si, and U in the REDOX process HLW, all the other analytes partitioned to some extent between solid and liquid phases.

5. Essentially all solid sodium salts, i.e., salt cake, added to the tank in 1965 dissolved in water and other aqueous solutions which were subsequently added to tank 241-SX-112.

6. The concentration of analytes in the REDOX process sludge in tank 241-SX-112 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]).

7. The waste transaction history and waste volume information for tank 241-SX-112 provided in Brevick et al. (1994) is assumed to be correct.

8. Radiolysis of NO_3 to NO_2 and any additions of nitrite to wastes in tank 241-SX-112 for corrosion control purposes are not accounted for in this independent assessment.

9. The mass of solid waste estimated by Agnew et al. (1997) to be present in tank 241-SX-112 is assumed to be correct.

D3.4 PREDICTED INVENTORY OF ANALYTES IN TANK 241-SX-112

The contributions to inventory from REDOX process HLW, which are determined by two different methods, follows.

D3.4.1 Application of Analytical Data for Wastes in Tanks 241-S-101, 241-S-104, and 241-S-107

Table D3-3 lists concentration data determined for samples of sludge from tanks 241-S-101, 241-S-104, and 241-S-107. Also listed in Table D3-3 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. 1997). 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 HLW sludge in tank 241-SX-112.

The inventory of various analytes in tank 241-SX-112 is calculated by multiplying each of the average analyte concentrations listed in Table D3-3 by 6.07 E+05 kg, the mass of solid waste stated (Agnew et al. 1997) to be in tank 241-SX-112. Results of these computations are shown in Table D3-4.

Table D3-3. R1 Sludge Concentration Estimate. (3 Sheets)

Analyte	241-S-101 segments 7U-8L[a] (μg/g)	241-S-104 (total sludge concentration[b] (μg/g)	241-S-107 segments [c] (μg/g)	Average concentration[d] (μg/g)	HDW sludge layer concentration[e]
Al	127,000	117,000	56,400	100,000	99,000
Ag	9.71	<DL	<DL	9.7	NR
B	63.1	26.6	49	46.2	NR
Bi	<38.8	<45.7	NR	<42.2	0.206
Ca	322	247	234	268	6,030
Cl	2,050	3,200	1,860	2,370	1,480

Table D3-3. R1 Sludge Concentration Estimate. (3 Sheets)

Analyte	241-S-101 segments 7U-8L[a] (μg/g)	241-S-104 (total sludge concentration[b] (μg/g)	241-S-107 segments [c] (μg/g)	Average concentration[d] (μg/g)	HDW sludge layer concentration[e]
Cr	2,230	2,350	1,180	1,920	7,560
F	<65.7	145	150	<120	0.966
Fe	1,960	1,720	1,160	1,613	39,100
Hg	NR	<0.126	NR	<0.126	
K	539	300	457	432	372
La	<19.5	<2.07	NR	<10.8	
Mn	2,750	1,150	83	1,330	0.394
Na	112,000	121,000	60,400	97,800	67,000
Ni	90.7	56	206	118	2,020
NO_2	31,100	25,900	34,300	30,433	42,100
NO_3	119,000	191,000	57,600	122,500	137,000
Pb	37	29.6	33	33.2	5.09
PO_4	1,360	<2,190	1,630	<1,730	6.06
P	278	93.2	391	254	NR
S	343	472	293	369	NR
Si	1,360	1,330	1,060	1,250	2,670
SO_4	897	2,270	1,300	1,489	1,100
Sr	456	424	378	420	0
TIC as CO_3	NR	4,140	NR	4,140	
TOC	NR	1,730	NR	1,730	12.9
U	7,684	6,690	8,685	7,690	617
Zn	25.1	NR	2.4	23.1	NR
Zr	36	33.6	131	66.9	0.00898
density (g/mL)	1.77	1.64	1.90	1.77	1.74

Table D3-3. R1 Sludge Concentration Estimate. (3 Sheets)

Analyte	241-S-101 segments 7U-8L[a] (μg/g)	241-S-104 (total sludge concentration[b] (μg/g)	241-S-107 segments [c] (μg/g)	Average concentration[d] (μg/g)	HDW sludge layer concentration[e]
Radionuclides[f] (μCi/g)					
^{90}Sr	NR	301	276	288	2,240
^{137}Cs	98[g]	60.5	74	77.6	103

NR = Not reported
HDW = Hanford Defined Waste
< DL = Less than the detectable limit
[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)
[f] Radionuclides decayed to January 1, 1994.

D3.4.2 Alternative Calculation Method for Inventory of Analytes Assumed to Completely Precipitate

Inventories of iron, manganese, bismuth, and uranium added to tank 241-SX-112 were calculated separately for 1956 to 1957, 1960 to 1961, and 1966.

These calculations utilized data presented in Tables D3-1 and D3-2. Inventories (kg) of each analyte were calculated as the product of the following factors:

- Volume (kgal) of waste slurry added to tank in respective times periods (Table D3-1)
- Molarity of analyte in waste stream (Table D3-2)
- Atomic weight of analyte (g)
- 1.0 E+03 gal/kgal--conversion factor

- 3.785 L/gal--conversion factor
- Kg/1.0 E+03 g--conversion factor

Results of these calculations are summarized below; in all cases, quantities are given as kg.

1956-57

Iron:	1,001 kgal x 0.0074 mole/L x 3.785 L/gal x 1.0 E+03 gal/kgal x kg/1.0 E+03 g x 55.85 g/mole = 1,566 kg
Manganese:	696 kg
Uranium:	3,340 kg

1960-61:

Iron:	807 kgal x 0.0075 mole/L x 3.785 L/gal x 1.0 E+03 gal/kgal x kg/1.0 E+03 g x 55.85 g/mole = 1,279 kg
Bismuth:	31.3 kg
Uranium:	480 kg

1966

Iron:	639 kgal x 0.016 mole/L x 3.785 L/gal x 1.0 E+03 gal/kgal x kg/1.0 E+03 g x 55.85 g/mole = 2,161 kg
Bismuth:	38.4 kg
Uranium:	466 kg

Total inventories of precipitable metals calculated by the alternate inventory determination method are:

Iron:	5,006 kg
Bismuth:	69.7 kg
Manganese:	696 kg
Uranium:	4,286 kg

The inventory value calculated for manganese is in good agreement with the value listed in Table D2-1. Such agreement supports use of the average of analyte concentration data for tanks 241-S-101, 241-S-104, and 241-S-107 to estimate the inventory of analytes in the sludge in tank 241-SX-111. On the other hand, the calculated bismuth and uranium inventories are two to three times the values listed in Table D3-4. No explanation can be offered for the difference in the two bismuth inventory values.

The real problem is with the widely different iron inventory estimates: 977 kg listed in Table D3-4 and 5,000 kg calculated from waste volumes and iron concentrations. There are many possible reasons for the difference in iron inventories: flowsheet iron concentrations too high, iron not completely precipitated, faulty analyses for iron in sludges in tanks 241-S-101, 241-S-104, and 241-S-107, etc. Apparently, the only way to resolve the issue is to sample and analyze sludge from tank 241-SX-112.

Comments and observations concerning comparison of HDW model and independent assessment inventory predictions for various analytes are also made in this section.

Caveat

The HDW model inventory predictions for tank 241-SX-112 were made on the basis that the solids now in the tank originated from REDOX process HLW and REDOX process salt cake. On the other hand, independent engineering assessments were made on the basis that solids in the tank originated from REDOX process HLW. This difference in prediction bases should always be kept in mind when comparing HDW model predictions to independent assessment values.

Inventory Comparisons

The HDW and the engineering assessment inventories are compared in Table D3-4 and in the observations that follow the table.

Table D3-4. Estimated Analyte Inventories for tank 241-SX-112. (2 Sheets)

Analyte	HDW model[a] (kg)	Independent assessment[b] (kg)
Nonradioactive		
Al	60,600	60,700
Bi	0.125	<25.6
Ca	3,660	163
Cl	899	1,440
TIC as CO_3	5,510	2,510
Cr	4,590	1,170
F	0.586	<72.9
Fe	23,700	977
Hg	0.0188	<0.076
K	226	262
La	2.05 E-07	<6.56
Mn	0.239	807

Table D3-4. Estimated Analyte Inventories for tank 241-SX-112. (2 Sheets)

Analyte	HDW model[a] (kg)	Independent assessment[b] (kg)
Na	67,000	59,400
Ni	1,230	71.6
NO_2	25,500	18,500
NO_3	82,900	74,400
OH	156,000	NR
Pb	3.09	20.2
PO_4	3.68	< 1,050
Si	1,620	759
SO_4	666	904
Sr	NR	255
TOC	7.8	1,050
Zr	0.00545	40.5
Radioactive[c]		
^{90}Sr	1.36 E+06	175,000
^{137}Cs	62,300	47,100
^{239}Pu	223 Ci	NR
^{238}U	0.127 Ci (374 kg)	1.57 Ci (4,670)

HDW = Hanford Defined Waste
NR = Not reported
[a] Agnew et al. (1997)
[b] This Tank Characterization Report
[c] Decayed to January 1, 1994; inventory of 44 other radionuclides presented in a later table.

Observations

Aluminum. The HDW model prediction of the aluminum content of tank 241-SX-112 is in excellent agreement with that predicted by the independent assessment (60,600 kg versus 60,800 kg). Such agreement is somewhat surprising since different bases for predicting the waste content of the tank were used for each method; apparently, the two prediction bases are not as different as one might expect. The independent assessment prediction is used as the best-basis inventory value.

Silver, Boron, Phosphorus, Sulfur, Nonradioactive Strontium, TOC (Total Organic Carbon, and Zinc. The amounts of these analytes in tank 241-SX-112 were not determined in the HDW model inventory assessment. Therefore, the independent assessment predictions are listed in Table D4-1 as the best-basis estimate.

Bismuth. The HDW model predicts tank 241-SX-112 to only contain 0.125 kg of bismuth. This result cannot be possibly correct since much of the REDOX process HLW introduced into the tank contained a small, but measurable, concentration of bismuth. Perhaps the HDW model value represents a calculation error. In any event, the engineering assessment leads to a value of <25.6 kg of bismuth in tank 241-SX-112; this latter value appears very reasonable.

Chromium. The HDW model predicts the waste in tank 241-SX-112 to contain about four times as much chromium as does the independent assessment. This difference reflects, to some extent, the difference in the amounts of chromium in REDOX process HLW assumed to partition to the solid phase. Also, in the HDW model a significant amount of chromium was contributed to the solids in the tank from the REDOX process salt cake assumed to be present in the tank; the independent assessment is made on the basis that REDOX process salt cake is not present in tank 241-SX-112. The 1,170 kg value is accepted as the best-basis inventory estimate.

Iron. The independent assessment value for the inventory of iron in tank 241-SX-112 is only about one-twenty fifth the amount predicted to be in the tank by the HDW model. The HDW model assumes that the concentration of iron in the REDOX process HLW added to the tank was a factor of five to six times higher than the published Flowsheet 5 and 6 values, 0.048*M* versus 0.0075*M*. The value of 977 kg iron is selected as the best-estimate inventory number even though a separate analysis, based upon the volume of waste added to the tank and the estimated concentration of iron in the waste, indicates that the iron content of tank 241-SX-112 could be as high as 5,000 kg.

Manganese. The HDW model (Rev. 4) predicts that tank 241-SX-112 contains only 0.239 kg of manganese. This value is absurdly low considering the presence of at least 0.0034*M* manganese in most of the REDOX process HLW added to the tank. The 0.239 kg value either reflects an incorrect calculation or an erroneous assumption about the solubility of manganese. Manganese surely would have precipitated when REDOX process HLW was made alkaline. The best-estimate value for the manganese inventory of tank 241-SX-112 is 807 kg, a value derived in the independent assessment.

Nickel. The independent assessment predicts only 71.6 kg of nickel in tank 241-SX-112 whereas the HDW model prediction is 1,230 kg. The HDW model nickel inventory reflects an incorrect assumption concerning the amount of corrosion of stainless steel equipment in the REDOX plant.

Nitrate. The independent assessment predicts tank 241-SX-112 to contain only slightly less nitrate as predicted by the HDW model (74,400 kg versus 82,900 kg). This development is quite surprising since the salt cake assumed to be present in the HDW model analysis should have contributed much nitrate. The independent assessment value of 74,400 kg nitrate is taken as the best-basis estimate.

Potassium. The independent assessment predicts tank 241-SX-112 to contain 262 kg of potassium, whereas, the HDW model predicts 226 kg of potassium are present. The principal reason for the difference is that the HDW model did not take into account potassium added as $KMnO_4$. The independent assessment value of 262 kg is selected as the best-basis estimate of the inventory of potassium in tank 241-SX-112.

Sodium. The independent engineering assessment predicts tank 241-SX-112 to contain only a factor of 1.1 less sodium than predicted by the HDW model. This result which parallels the situation with the nitrate content of this tank is surprising since the expectation is that salt cake, assumed to be present in the HDW model base assumption, would contain considerable amounts of both sodium and nitrate. In any event, the engineering assessment value of 59,400 kg sodium is taken as the best-basis estimate.

Sulfate. The sulfate content of the solids in tank 241-SX-112 as determined by the independent engineering assessment is 904 kg. This value is in reasonable agreement with the value of 666 kg of sulfate as predicted by the HDW model. Such agreement must be considered fortuitous considering that different prediction bases were used in the two prediction approaches. The value of 904 kg of sulfate is chosen as the best-basis estimate.

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. No such adjustments were needed in this tank. This charge balance approach is consistent with that used by Agnew et al. (1997).

Uranium. The HDW model predicts the waste in tank 241-SX-112 to only contain 0.127 Ci (374 kg) of uranium, whereas, the independent assessment, based upon the average analytically determined uranium content of sludges in tanks 241-S-101, 241-S-104, and 241-S-107, predicts tank 241-SX-112 to contain 4,670 kg of uranium. On the other hand, an engineering assessment based upon the volume of REDOX process HLW added to the tank leads to a calculated uranium inventory of 4,290 kg. The value of 4,670 kg uranium is selected as the best-basis inventory estimate.

D4.0 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-SX-112 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)
- Average of analyte concentrations in REDOX process HLW sludges in tanks 241-S-101, 241-S-104, and 241-S-107
- Inventory estimates generated by a tank-specific assessment process utilizing chemical process flowsheets and a detailed historical tank waste transaction data base.

The results from this evaluation support using a predicted inventory based primarily on results from a tank-specific assessment process utilizing the average of analyte concentrations for REDOX process waste sludges in tanks 241-S-101 (Kruger et al. [1996]), 241-S-104 (DiCenso et al. [1994]), and 241-S-107 (Simpson et al. [1996]) for the following reasons:

1. The waste in tank 241-SX-112 has not been analyzed; it is not possible to use a predicted inventory based on analytical results.
2. The tank-specific assessment correctly predicts, based upon a careful and meticulous review of historical waste transaction records, that only REDOX process HLW of all the wastes introduced into tank 241-SX-112, contributed to the solid waste in the tank.
3. The HDW model incorrectly attributes part of the solids now in tank 241-SX-112 to salt cake precipitated from one addition of concentrated REDOX process HLW supernatant. Such analysis ignores the large volumes of water that were added to the tank subsequent to precipitation of any salt cake solids. Experimental evidence exists (Schulz 1980) that strongly suggests any precipitated salt cake would have readily dissolved.

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 D4-1 and D4-2 are subject to change. Refer to the Tank Characterization Database (TCD) for the most current inventory values.

Table D4-1. Best-Basis Inventory Estimates for Nonradioactive Components in Tank 241-SX-112 (Effective March 10, 1997).

Analyte	Total inventory (kg)	Basis (S, M, E, or C)[1]	Comment
Al	60,700	E	
Bi	<25.6	E	
Ca	163	E	
Cl	1,440	E	
TIC as CO_3	2,510	E	
Cr	1,170	E	
F	<72.9	E	
Fe	977	E	
Hg	<0.076	E	
K	262	E	
La	<6.56	E	
Mn	807	E	
Na	59,400	E	
Ni	71.6	E	
NO_2	18,500	E	
NO_3	73,400	E	
OH_{TOTAL}	133,000	C	
Pb	20.2	E	
PO_4	<1,050	E	
Si	759	E	
SO_4	904	E	
Sr	255	E	
TOC	1,050	E	
U_{TOTAL}	4,670	E	
Zr	40.5	E	

[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 D4-2. Best-Basis Inventory Estimates for Radioactive Components in Tank 241-SX-112, Decayed to January 1, 1994 (Effective March 10, 1997). (2 Sheets)

Analyte	Total inventory (Ci)	Basis (S, M, or E)[1]	Comment
^{3}H	38.2	M	
^{14}C	1.97	M	
^{59}Ni	10.7	M	
^{60}Co	1.71	M	
^{63}Ni	1,050	M	
^{79}Se	3.98	M	
^{90}Sr	175,000	E	
^{90}Y	175,000	E	Referenced to ^{90}Sr
^{93}Zr	17.0	M	
^{93m}Nb	15.7	M	
^{99}Tc	15.3	M	
^{106}Ru	3.89 E-04	M	
^{113m}Cd	7.95	M	
^{125}Sb	6.01	M	
^{126}Sn	5.21	M	
^{129}I	0.0290	M	
^{134}Cs	0.435	M	
^{137}Cs	47,100	E	
^{137m}Ba	44,600	E	Referenced to ^{137}Cs
^{151}Sm	14,300	M	
^{152}Eu	12.5	M	
^{154}Eu	41.3	M	
^{155}Eu	636	M	
^{226}Ra	9.22 E-04	M	
^{227}Ac	0.00416	M	
^{228}Ra	0.00137	M	
^{229}Th	3.43 E-05	M	
^{231}Pa	0.00447	M	
^{232}Th	1.84 E-05	M	
^{232}U	0.00613	M	

Table D4-2. Best-Basis Inventory Estimates for Radioactive Components in Tank 241-SX-112, Decayed to January 1, 1994 (Effective March 10, 1997). (2 Sheets)

Analyte	Total inventory (Ci)	Basis (S, M, or E)[1]	Comment
^{233}U	0.0234	M	
^{234}U	0.144	M	
^{235}U	0.00583	M	
^{236}U	0.00580	M	
^{237}Np	0.0683	M	
^{238}Pu	8.42	M	
^{238}U	1.57	E	
^{239}Pu	223	M	
^{240}Pu	39.0	M	
^{241}Am	220	M	
^{241}Pu	418	M	
^{242}Cm	0.529	M	
^{242}Pu	0.00232	M	
^{243}Am	0.00972	M	
^{243}Cm	0.0514	M	
^{244}Cm	1.54	M	

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

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D5.0 APPENDIX D REFERENCES

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