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Preliminary Tank Characterization Report for Single-Shell Tank 241-SX-101: 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-101 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-101: BEST-BASIS INVENTORY

August 1997

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PRELIMINARY TANK CHARACTERIZATION REPORT FOR SINGLE-SHELL TANK 241-SX-101: 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-101. 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 (W²S 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.

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APPENDIX D

EVALUATION TO ESTABLISH BEST-BASIS INVENTORY FOR SINGLE-SHELL TANK 241-SX-101

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APPENDIX D

EVALUATION TO ESTABLISH BEST-BASIS INVENTORY FOR SINGLE-SHELL TANK 241-SX-101

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 tank 241-SX-101 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.

D1.0 CHEMICAL INFORMATION SOURCES

There is no previous Tank Characterization Report (TCR) for single-shell tank (SST) 241-SX-101. Available waste (chemical) information for tank 241-SX-101 includes the following:

- Analytical data for other S and U tanks with similar salt cake and sludge waste type.
- The Hanford Defined Waste (HDW) model document (Agnew et al. 1996) provides tank content estimates.

D2.0 COMPARISON OF COMPONENT INVENTORY VALUES

HDW model inventories are shown in Tables D2-1 and D2-2. No samples have been taken from tank 241-SX-101 that can be used to estimate tank inventories for comparison with the HDW model. The tank volume used to generate the HDW inventory is 1,726 kL (456 kgal) waste which is partitioned into 583 kL (154 kgal) sludge and 1,139 kL (301 kgal) salt cake (Agnew et al. 1996). This differs from the 1,726 kL (456 kgal) total waste of which 424 kL (112 kgal) is sludge, 1,298 kL (343 kgal) is salt cake, and 3.78 kL (1 kgal) is supernatant reported by (Hanlon 1996). It should be noted that the 3.78 kL (1 kgal) of supernate reported by Hanlon was not included in these calculations. The amount that may be in the supernate is a small amount and will cause only a small error in determining this estimate. (The chemical species are reported without charge designation per the best-basis inventory convention.)

Table D2-1. Hanford Defined Waste-Based Inventory Estimates for Nonradioactive Components in Tank 241-SX-101. (2 Sheets)

Analyte	HDW[a] inventory estimate (kg)	Analyte	HDW[a] inventory estimate (kg)
Al	97,300	NO_3	272,000
Bi	64.8	OH	276,000
Ca	7,160	oxalate	0.666
Cl	5,000	Pb	70.5
Cr	34,200	P as PO_4	2,060
F	332	Si	2,870
Fe	33,600	S as SO_4	8,900
Hg	0.560	Sr	0.258
K	1,300	TIC as CO3	16,600
La	1.23	TOC	3,060
Mn	52.1	U_{TOTAL}	8,470
Na	217,000	Zr	19.5
Ni	2,350	H_2O (Wt%)	55.2
NO2	129,000	density (kg/L)	1.41

HDW = Hanford Defined Waste
[a] Agnew et al. (1996).

Table D2-2. Predicted Inventory Estimates for Radioactive Components in Tank 241-SX-101.

Analyte	HDW[a] inventory estimate (Ci)	Analyte	HDW[a] inventory estimate (Ci)
^{90}Sr	793,000	$^{239/240}Pu$	115
^{137}Cs	280,000		

HDW = Hanford Defined Waste
[a] Agnew et al. (1996), decayed to January 1, 1994.

D3.0 COMPONENT INVENTORY EVALUATION

D3.1 WASTE HISTORY TANK 241-SX-101

Tank 241-SX-101 was filled with waste from the Reduction and Oxidation (REDOX) facility from the second quarter of 1954 until the third quarter of 1971. Tank 241-SX-101 received 15,660 kL (4,136 kgal) of first-cycle REDOX (R1) process waste during 1954 and 1955. A total of 4,670 kL (1,234 kgal) of the R1 waste cascaded into tank 241-SX-102. From 1972 until the tank was removed from service, 241-SX-101 sent and received waste from the 242-S evaporator. The tank was removed from service in 1980 and was partially isolated in June 1985.

D3.2 EVALUATION OF TANK WASTE VOLUME

Tank 241-SX-101 is categorized as sound and is partially isolated. The Tank 241-SX-101 surface level was monitored with a Food Instrument Corporation gauge through riser 4 until it was replaced with an ENRAF (not an acronym, but the capitalized name of the manufacturer) gauge in 1995. Due to the Food Instrument Corporation gauge setting, a limited number of surface level measurements are available during its operation. As of January 16, 1997, the ENRAF surface level reading was 409.4 cm (161.19 in.), which correlates to 1,624 kL (429 kgal) of total waste.

D3.3 CONTRIBUTING WASTE TYPES

The HDW model (Agnew et al. 1996) predicts that the tank contains a total of 1,726 kL (456 kgal) of waste which consists of 583 kL (154 kgal) REDOX process high-level waste (R1), 590 kL (156 kgal) REDOX process salt cake (R SltCk), and 549 kL (145 kgal) of salt cake: 352 kL (93 kgal) Supernatant Mixing Model 242-S Evaporator salt cake generated from 1973 until 1976 (SMMS1) and 197 kL (52 kgal) Supernatant Mixing Model 242-S Evaporator salt cake generated from 1977 until 1980 (SMMS2).

The Sort on Radioactive Waste Type (SORWT) model (Hill 1995) lists R (high-level REDOX process waste), and Evaporator Bottoms (EB) as the primary and secondary waste types respectively. EB waste is the SORWT definition for salt cake that is equivalent to the SMM waste type. Hill also lists REDOX process ion exchange waste as a tertiary contributor.

Hanlon (1996) indicates 1,726 kL (456 kgal) of waste which consists of 424 kL (112 kgal) of sludge and 1,298 kL (343 kgal) of salt cake. No description of the source of the sludge and salt cake are given.

D3.4 ASSUMPTIONS USED

For this evaluation, the following assumptions and observations are made:

- Tank waste volume listed in Hanlon (1996) is 1,726 kL (456 kgal) which is in good agreement with the ENRAF surface level data of 1,624 kL (429 kgal) total waste.

- Only the SMMS1, SMMS2, R SltCk, and REDOX (R) process waste streams contributed to solids formation.

- The Hanlon volumes for salt cake and sludge was assumed. The sludge is assumed to be 424 kL (112 kgal) REDOX (R). The 1298 kL (343 kgal) R StlCk, SMMS1 and SMMS2 is represented by 832 kL (220 kgal) SMMS1, and 455 kL (123 kgal) SMMS2. These ratios are based on the volume ratios for SMMS1 and SMMS2 on Appendix C of Agnew et al. 1996, for tank 241-SX-101.

D3.5 BASIS FOR CALCULATIONS USED IN THIS ENGINEERING EVALUATION

Table D3-1 shows the engineering evaluation approaches used on tank 241-SX-101.

Table D3-1. Engineering Evaluation Approaches Used On 241-SX-101.

Type of waste	How calculated	Check method
Supernatant	Assumed no supernatant	None, even though Hanlon indicates 3.8 kL (1,000 gal) supernate, no method is available to calculate its contribution to the inventory.
Salt cake Volume = 1,298 kL (343 kgal) Density = 1.63 g/ml for SMMS1 and 1.56 g/ml for SMMS2 waste.	Used sampling based concentrations from tanks with SMMS1 and/or SMMS2 waste types. SMMS1 = 832 kL (230 kgal) SMMS2 = 466 kL (123 kgal)	None, no sampling based information is available for this tank.

Table D3-1. Engineering Evaluation Approaches Used On 241-SX-101.

Type of waste	How calculated	Check method
Sludge Volume = 424 kL (112 kgal) Density = 1.77 g/ml	Used the average analyte concentration from tank 241-S-102, 241-S-104, and 241-S-107. All have sample data and R1 waste. Only the segments that are believed to have R1 waste were used to calculate the concentration from each tank.	None, no sampling based information is available for this tank.

D3.5.1 Basis for Salt Cake Calculations Used in this Engineering Evaluation

For this evaluation the methodology developed for SMMS1 and SMMS2 salt cake was used. This is based on comparing concentrations from S and U Tank Farm sample data shown in Table D3-2 and D3-3. Tanks 241-S-101, 241-S-102, 241-U-106, and 241-U-109 (Kruger et al. 1996, Eggers et al. 1996, Brown et al. 1997, and Baldwin and Stephens 1996) were used to produce the average salt cake analyte concentrations for SMMS1 salt cake and tanks 241-S-101, 241-S-102, 241-U-102, 241-U-107, and 241-U-109 (Kruger et al. 1996, Eggers et al. 1996, Hu et al. 1997, and Jo et al. 1996) for SMMS2 salt cake were used in this comparison. To calculate the average SMMS1 and SMMS2 concentration the waste volumes and predicted location from Agnew et al. (1996) for both the SMMS1 and SMMS2 layers in each tank were determined. The analytical data from the tanks listed above were reviewed and using the segments that were located within the predicted location from Agnew et al., an average concentration was calculated. The concentrations from each tank and the segments used in the calculation are shown in Table D3-2 and D3-3. For comparison the SMM salt cake composition predicted by the HDW model for tank 241-SX-101 is also shown.

Table D3-2. SMMS1 Salt Cake Concentrations. (2 Sheets)

Analyte	241-S-101 segments 2L-4U[a] (μg/g)	241-S-102 segments 7L-10U[b] (μg/g)	241-U-106 segments 2U-4L[c] (μg/g)	241-U-109 segments 5U-8L[d] (μg/g)	Average conc.[e] (μg/g)	HDW model SMM conc. for tank 241-SX-101[f] (μg/g)
Al	18,000	15,085	13,620	13,625	15,100	15,200
Ag	12	17	16	NR	15	NR
B	110	75	80	NR	88	NR
Bi	71	76	<DL	<DL	73.5	93.3
Ca	273	237	336	<DL	282	484
Cl	4,500	4,099	2,926	NR	3,842	2,570
Cr	10,000	4,359	3,170	4,233	5,440	1,110
F	500	13,596	4,669	NR	6,255	2,570
Fe	508	1,298	3,096	<DL	1,630	148
K	1,109	898	1,309	NR	1,110	757
La	<DL	37	43	NR	40	1.79
Mn	266	597	1,189	<DL	684	73.5
Na	150,000	189,500	170,500	218,300	182,000	94,500
Ni	114	49	304	<DL	155	NR
NO_2	91,000	40,100	56,000	42,900	57,500	39,000
NO_3	110,000	99,200	147,200	297,000	163,000	113,000
Pb	91	137	348	NR	192	69.4
PO_4	9,500	114,500	5,888	5,970	34,000	2,960
P	2,290	33,900	1,949	<DL	12,700	NR
S	5,940	2,683	3,878	NR	4,170	NR
Si	5,269	517	176	<DL	1,990	786
SO_4	20,700	12,500	10,774	11,100	13,800	8,090
Sr	7	<DL	<DL	NR	7	0.377
TOC	1,900	5,340	24,626	3,920	8,950	NR
U	560	1,403	781	<DL	914	1,040
Zn	30	32	54	<DL	39	NR
Zr	14	39	88	NR	47	28.2
Oxalate	15,400	15,700	9,880	NR	13,700	0.972

Table D3-2. SMMS1 Salt Cake Concentrations. (2 Sheets)

Analyte	241-S-101 segments 2L-4U[a] (μg/g)	241-S-102 segments 7L-10U[b] (μg/g)	241-U-106 segments 2U-4L[c] (μg/g)	241-U-109 segments 5U-8L[d] (μg/g)	Average conc.[e] (μg/g)	HDW model SMM conc. for tank 241-SX-101[f] (μg/g)
Density g/mL	1.58	1.69	1.57	1.67	1.63	1.24
Radionuclides[g] (μCi/g)						
^{90}Sr	252	23	77	9	90	42.9
^{137}Cs	175	121	175	142	153	90.5

<DL = Less then the Detectable Limit.
HDW = Hanford Defined Waste
NR = Not reported
SMMS1 = Supernatant Mixing Model 242-S Evaporator salt cake generated from 1973 until 1976
[a] Kruger et al. (1996)
[b] Eggers et al. (1996)
[c] Brown et al. (1997)
[d] Baldwin and Stephens (1996)
[e] Average of tank 241-S-101, 241-S-102, 241-U-106, and 241-U-109 concentrations
[f] Agnew et al. (1996)
[g] Radionuclides are reported as of the date of sample analysis.

Table D3-3. SMMS2 Salt Cake Concentrations (Average from Tanks with Tank Characterization Reports). (2 Sheets)

Analyte	241-S-101 segments 1U-2U[a] (µg/g)	241-S-102 segments 2U-5L[b] (µg/g)	241-U-102 segments 2U[c] (µg/g)	241-U-107 segments 2U-6L[d] (µg/g)	241-U-109 segments 1L-4U[e] (µg/g)	Average conc.[f] (µg/g)	HDW model SMM conc. for tank 241-SX-101[g] (µg/g)
Al	16,925	7,450	10,505	10,612	9,487	10,966	15,200
Ag	12	17	13	16	NR	14	NR
B	111	58	67	89	NR	81	NR
Bi	51	<DL	<DL	270	<DL	161	93.3
Ca	274	233	310	298	<DL	279	484
Cl	4,607	2,981	4,550	2,515	3,560	3,643	2,570
Cr	8,163	1,577	2,417	2,570	2,570	3,456	1,110
F	638	267	896	501	299	520	2,570
Fe	453	65	565	767	1,630	696	148
K	1,225	748	1,360	914	NR	1,062	757
Mn	541	26	137	330	<DL	258	73.5
Na	153,000	207,000	176,000	205,667	237,333	195,800	94,500
Ni	115	19	77	56	<DL	67	NR
NO_2	58,150	28,939	36,250	27,600	42,900	38,800	39,000
$3NO_3$	218,500	514,000	293,000	455,333	407,333	377,633	113,000
Pb	66	47	<DL	149	NR	87	69.4
PO_4	9,230	15,589	19,950	13,509	5,970	12,800	2,960
P	2,333	2,860	6,187	2,580	7,780	4,348	NR
S	4,713	1,325	4,037	1,090	NR	2,791	NR
Si	<DL	219	148	194	1,220	445	786
SO_4	21,185	8,553	12,785	4,112	11,000	11,530	8,090
Sr	48	<DL	<DL	9	NR	28	0.337
TOC	NR	1,898	6,417	2,414	2,330	3,260	NR
U	1,497	<DL	<DL	430	<DL	964	1,040
Zn	33	21	33	29	NR	29	NR
Zr	13	<DL	<DL	13	NR	13	28.3

Table D3-3. SMMS2 Salt Cake Concentrations (Average from Tanks with Tank Characterization Reports). (2 Sheets)

Analyte	241-S-101 segments 1U-2U[a] (μg/g)	241-S-102 segments 2U-5L[b] (μg/g)	241-U-102 segments 2U[c] (μg/g)	241-U-107 segments 2U-6L[d] (μg/g)	241-U-109 segments 1L-4U[e] (μg/g)	Average conc.[f] (μg/g)	HDW model SMM conc. for tank 241-SX-101[g] (μg/g)
Radionuclide[h] (Ci)							
^{90}Sr	252	NR	<DL	0.297	4.81	86	42.9
^{137}Cs	160.15	NR	136.5	62.06	89.1	112	90.5

<DL = Less than detectable limit
HDW = Hanford Defined Waste
NR = Not reported
SMMS2 = Supernatant Mixing Model 242-S Evaporator salt cake generated from 1977 until 1980
[a] Kruger et al. (1996)
[b] Eggers et al. (1996)
[c] Hu et al. (1997)
[d] Jo et al. (1996)
[e] Baldwin and Stephens (1996)
[f] Average of tank 241-S-101, 241-S-102, 241-U-102, 241-U-107, and 241-U-109 concentrations
[g] Agnew et al. (1996)
[h] Radionuclides are reported as of the date of sample analysis.

D3.5.2 Basis for Sludge Calculations Used In This Engineering Evaluation.

Data from tanks 241-S-102, 241-S-104, and 241-S-107 (Kruger et al. 1996, DiCenso et al. 1994, Simpson et al. 1996) were used to produce average analyte concentrations for R1 sludge waste. To calculate the average concentration, the volumes and predicted location of the sludge were taken from Agnew et al. (1996) for the tanks R1 waste. The sample data were then reviewed, and only the segments that were located within the predicted sludge location from Agnew et al. were used in deriving an average concentration. The average concentration from each tank and the segments used in the calculation is shown below in Table D3-4. For comparison the average sludge layer composition predicted by the HDW model for tank 241-SX-101 is also shown.

Table D3-4. R1 Sludge Concentrations μg/g (Average from Tanks with Tank Characterization Reports) for Tank 241-SX-101. (2 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 Model Sludge Values for 241-TX-101[e] (μg/g)
Al	127,000	117,000	56,400	100,000	49,800
Bi	< 38.8	<45.7	NR	< 42.2	NR
Ca	322	247	234	268	NR
Cl	2,050	3,200	1,860	2,370	0.534
Cr	2,230	2,350	1,180	1,920	3,910
F	<65.7	145	150	<120	1,860
Fe	1,960	1,720	1,160	1,613	19,200
Hg	NR	<0.126	NR	<0.126	2.78
K	539	300	457	432	19,200
La	<19.5	<2.07	NR	<10.8	NR
Mn	2,750	1,150	83	1,330	1.02
Na	112,000	121,000	60,400	97,800	87,100
Ni	90.7	56	206	118	NR
NO_2	31,100	25,900	34,300	30,433	85,900
NO_3	119,000	191,000	57,600	122,500	112,000
Pb	37	29.6	33	33.2	13.2
PO_4	1,360	<2,190	1,630	<1,730	15.6
Si	1,360	1,330	1,060	1,250	1,330
SO_4	897	2,270	1,300	1,489	1,930
Sr	456	424	378	420	2.64E-06
TIC as CO_3	NR	4,140	NR	4,140	3,060
TOC	NR	1,730	NR	1,730	4,440
U	7,684	6,690	8,685	7,690	2.71 E+0
Zr	36	33.6	131	66.9	0.113
Radionuclides (μCi/g)					
^{90}Sr	NR	301[f]	276[f]	288[f]	326
^{137}Cs	98[f]	60.5[f]	74[f]	77.6[f]	115

Table D3-4. R1 Sludge Concentrations μg/g (Average from Tanks with Tank Characterization Reports) for Tank 241-SX-101. (2 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 Model Sludge Values for 241-TX-101[e] (μg/g)
density (g/ml)	1.77	1.64	1.90	1.77	1.41

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. (1996)
[f] Radionuclides decayed to January 1, 1994.

D3.6 ESTIMATED COMPONENT INVENTORIES

The Chemical inventory of tanks 241-SX-101 is estimated from the assumed salt cake and sludge volumes (Table D3-1). The resulting inventories are provided in Table D3-5. The inventories estimated by the HDW model are included for comparison.

Table D3-5. Comparison of Selected Component Inventory Estimates for Tank 241-SX-101. (2 Sheets)

Analyte	This evaluation (kg) Sludge	This evaluation (kg) Salt Cake	This evaluation (kg)	HDW[a] estimated (kg)
Bi	<31.7	217	<249	64.8
K	324	2,280	2,610	1,300
La	<8.1	54	<62.1	1.23
NO_3	91,900	495,000	587,000	272,000
Mn	998	1,120	2,110	52.1
SO_4	1,120	27,100	28,200	8,900
Cr	1,440	9,900	11,300	34,200
Ca	201	586	787	7,160

Table D3-5. Comparison of Selected Component Inventory Estimates for Tank 241-SX-101. (2 Sheets)

Analyte	This evaluation (kg) Sludge	This evaluation (kg) Salt Cake	This evaluation (kg)	HDW[a] estimated (kg)
Ni	88.5	261	349	2,350
PO_4	<1,300	55,500	56,800	2,060
F	90.0	6,850	6,940	332
Al	75,100	28,500	104,000	97,300
Fe	1,210	2,720	3,930	33,600
TOC	1,300	14,500	15,800	3,060
Na	73,400	389,000	462,400	217,000
H_2O (percent)	NR	28.4	28.4	55.2

HDW = Hanford Defined Waste
NR = Not reported
[a] Agnew et al. 1996.

Since no post-1989 analytical data were available from this tank, the reliability of these estimates (in either this engineering assessment or the HDW model inventory estimates) are suspect. Although these uncertainties cannot be resolved at this point, some trends can be discussed.

Manganese. Potassium permanganate was used in the REDOX process until 1959, thus manganese is expected to be found in tanks containing waste from that process. It is most likely present as highly insoluble manganese dioxide in the alkaline waste materials and would be expected to be in the sludge. The R1 Sludge composition estimate developed in this engineering assessment for Mn was 1,330 μg/g. Interestingly, the SMMS1 salt cake composition estimate for Mn was 684 μg/g - much higher than would be expected based on solubility considerations, and the SMMS2 salt cake composition estimate is 258 μg/g. It should be noted that there are large ranges in the SMMS1, SMMS2, and R1 data sets for Mn.

The HDW model predicts only 1.02 μg/g Mn in the Sludge in tank 241-SX-101 and 73.5 μg/g in the salt cake layer. The HDW model inventory estimate for Mn is 52.1 kg. Based on the discussion above, the 2,110 kg inventory estimate developed in this engineering assessment is likely to be closer to the true value.

Phosphate. There is a large difference between the engineering assessment tank inventory estimate (56,800 kg) and the HDW model estimate (2,060 kg). The engineering assessment value is biased high because of one extremely high phosphate value in data set used to develop the SMMS1 salt cake composition estimate (see Table D3-2). If the phosphate data from tank 241-S-102 are eliminated from the SMMS1 composition estimate then the engineering assessment and the HDW estimate would be in reasonable agreement. However, since the HDW model failed to predict the high phosphate value for 241-S-102, it should not be taken as a reliable indicator for phosphate in tank 241-SX-101.

Calcium. The calcium found in tanks containing REDOX process waste is believed to have been an impurity in the commercial grade sodium hydroxide used in the neutralization of high-level waste in the process. The calcium value developed in this engineering assessment (787 kg) is about one tenth of the HDW model value (7,160 kg). Since many calcium salts of anions such as carbonate, oxalate and phosphate are insoluble and the concentrations of these anions are essentially unknown, it is not surprising that Ca values differ between this engineering assessment and the HDW model.

Fluoride. The fluoride ion inventory estimate is over 21 times higher in the engineering assessment (6,940 kg) than in the HDW model (332 kg). However, as shown by the data in Table D3-2, the fluoride values in two of the four tanks agree with the HDW model value. The fluoride concentration in tanks 241-S-102 and 241-U-106 are much higher. Without analytical data from tank 241-SX-101, it is difficult to defend the choice of one value over the other.

Iron. The Fe inventory estimate is about almost an order of magnitude higher in the HDW model than in the engineering assessment. The Fe value determined in the engineering assessment for the salt cake is approximately 25 times the HDW model value. As shown in Table D3-2 and D3-3, the data set used to estimate Fe in the SMMS1 salt cake varies from 3,096 μg/g to less than detection limit and varies from 65 to 1,630 μg/g for the SMMS2 salt cake. The HDW model predicts over 99 percent of the tank Fe inventory to be in the sludge while the engineering assessment indicates less than 40 percent of the Fe total mass to be in the sludge. Without analytical data from tank 241-SX-101 it is difficult to defend the choice of one value over the other.

Sodium. The sodium value determined in this engineering assessment is approximately twice the value predicted by the HDW model. As shown in Table D3-2 and D3-3, the sodium values in the salt cake data from the four tanks are reasonably consistent. The reason for the two-fold difference is unclear.

Nickel. The nickel inventory from the engineering assessment is approximately one seventh the value of the HDW model inventory. The HDW model predicts the majority of the Ni to be in the sludge, this is where the major differences in the two evaluations is seen. The salt cake engineering assessment value and the SMM modeling from the HDW estimate agree very well with each other.

Total Hydroxide. Once the best-basis inventories were determined, the hydroxide inventory was calculated by performing a charge balance with the valence 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 retained. This charge balance approach is consistent with that used by Agnew et al. (1997).

D4.0 DEFINE THE BEST-BASIS AND ESTABLISH COMPONENT INVENTORIES

Key waste management activities include overseeing tank farm operations and identifying, monitoring and resolving safety issues associated with these operations and with the tank wastes. Disposal activities involve designing equipment, processes and facilities for retrieving wastes and processing them into a form that is suitable for long-term storage. Information about chemical, radiological and/or physical properties is used to perform safety analyses, engineering evaluations, and risk assessment associated with these activities.

Chemical and radiological inventory information are generally derived using three approaches: (1) component inventories are estimated using the results of sample analyses, (2) component inventories are predicted using the HDW model, process knowledge, and historical information, or (3) a tank-specific process estimate is made based on process flowsheets, reactor fuel data, essential material usage and other operating data.

As part of this effort, an evaluation of available chemical information for tank 241-SX-101 was performed, including the following:

- The inventory estimate generated by the HDW model (Agnew et al. 1996)

- An engineering evaluation which produced a predicted SMMS inventory and R1 sludge inventory based on methodology developed by evaluation of similar waste in the S and U tank farms.

Based on this evaluation, a best-basis inventory was developed for tank 241-SX-101 since sampling information is not available. The engineering evaluation inventory was chosen as the best basis for those analytes for which sampling-based analytical values were available, from similar S and U tank farm tanks, for the following reasons:

- The sampling-based inventory analytical concentrations of the other S and U tanks containing SMMS1 and SMMS2 compared favorably with each other for SMMS1 and SMMS2 salt cake

- No methodology is available to fully predict SMMS salt cake from process flowsheet or historical records

- No methodology is available to fully predict R1 waste from process flowsheet or historical records for this tank. REDOX process first-cycle R1 waste changed composition during the process and accurate records of these changes are not available at this time. Also R1 waste was cascaded and transferred into and out of many S, SX, and U tanks between 1972 and 1978 which makes it hard to predict precipitation factors for analytes in the waste. Some tanks will show higher concentrations for certain analytes because of the length of time the waste was in the tank before being transferred out.

- For those few analytes where no values were available from the sampling-based inventory of similar tanks.

The best-basis inventory for tank 241-SX-101 is presented in Tables D4-1 and D4-2. 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.

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 Hanford Defined Waste 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.

Best-basis tables for chemicals and only four radionuclides (^{90}Sr, ^{137}Cs, Pu and U) were being generated in 1996, using values derived from an earlier version (Rev. 3) of the Hanford Defined Waste model. When values for all 46 radionuclides became available in Rev 4 of the HDW model, they were merged with draft best-basis chemical inventory documents. Defined scope of work in FY 1997 did not permit Rev. 3 chemical values to be updated to Rev. 4 chemical values.

Table D4-1. Best-Basis Inventory Estimates for Nonradioactive Components in Tank 241-SX-101 (January 31, 1997).

Analyte	Total inventory (kg)	Basis (S, M, C, or E)[a]	Comment
Al	104,000	E	
Bi	<249	E	
Ca	787	E	
Cl	8,870	E	
TIC as CO_3	16,600	M	
Cr	11,300	E	
F	6,940	E	
Fe	3,910	E	
Hg	0.560	M	
K	2,610	E	
La	<62.1	E	
Mn	2,110	E	
Na	462,000	E	
Ni	349	E	
NO_2	129,000	E	
NO_3	587,000	E	
OH	280,000	C	
Pb	349	E	
P as PO_4	56,800	E	
Si	3,960	E	
S as SO_4	28,200	E	
Sr	345	E	
TOC	15,800	E	
U_{TOTAL}	7,710	E	
Zr	123	E	

[a]S = Sample-based
M = Hanford Defined Waste model-based, Agnew et al. (1996)
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-101 Decayed to January 1, 1994 (January 31, 1997). (2 Sheets)

Analyte	Total inventory (Ci)	Basis (S, M, or E)[a]	Comment
^{3}H	217	M	
^{14}C	17.7	M	
^{59}Ni	13.3	M	
^{60}Co	17.2	M	
^{63}Ni	1,260	M	
^{79}Se	5.35	M	
^{90}Sr	411,000	E	
^{90}Y	411,000	E	Based on ^{90}Sr
^{93}Zr	25.5	M	
^{93m}Nb	20.3	M	
^{99}Tc	131	M	
^{106}Ru	0.00329	M	
^{113m}Cd	56.2	M	
^{125}Sb	68.1	M	
^{126}Sn	8.19	M	
^{129}I	0.25	M	
^{134}Cs	2.09	M	
^{137}Cs	362,000	E	
^{137m}Ba	343,000	E	Based on ^{137}Cs
^{151}Sm	19,000	M	
^{152}Eu	10.4	M	
^{154}Eu	331	M	
^{155}Eu	523	M	
^{226}Ra	9.48 E-04	M	
^{227}Ac	0.00466	M	
^{228}Ra	0.0461	M	
^{229}Th	0.00109	M	
^{231}Pa	0.00772	M	
^{232}Th	0.00257	M	
^{232}U	0.233	M	

Table D4-2. Best-Basis Inventory Estimates for Radioactive Components in Tank 241-SX-101 Decayed to January 1, 1994 (January 31, 1997). (2 Sheets)

Analyte	Total inventory (Ci)	Basis (S, M, or E)[a]	Comment
^{233}U	0.894	M	
^{234}U	1.05	M	
^{235}U	0.0427	M	
^{236}U	0.0393	M	
^{237}Np	0.542	M	
^{238}Pu	5.64	M	
^{238}U	0.992	M	
^{239}Pu	333	M	
^{240}Pu	49.1	M	
^{241}Am	89.9	M	
^{241}Pu	329	M	
^{242}Cm	0.136	M	
^{242}Pu	0.00158	M	
^{243}Am	0.0028	M	
^{243}Cm	0.00598	M	
^{244}Cm	0.0395	M	

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

D5.0 APPENDIX D REFERENCES

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