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Preliminary Tank Characterization Report for Single-Shell Tank 241-S-103: 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-S-103 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-S-103: BEST-BASIS INVENTORY

August 1997

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U.S. Department of Energy
Richland, Washington

PRELIMINARY TANK CHARACTERIZATION REPORT FOR SINGLE-SHELL TANK 241-S-103: 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-S-103. 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-S-103

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APPENDIX D

EVALUATION TO ESTABLISH BEST-BASIS INVENTORY FOR SINGLE-SHELL TANK 241-S-103

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-S-103 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 this tank. Available waste (chemical) information for tank 241-S-103 includes the following:

- The inventory estimate for this tank generated from the Hanford Defined Waste (HDW) model (Agnew et al. 1996)
- TCRs from other tanks with the same Supernatant Mixing Model 242-S Evaporator salt cake generated from 1973 until 1976 (SMMS1) and from 1977 until 1980 (SMMS2) and Reduction and Oxidation (REDOX [R]) process sludge waste types (Baldwin 1996, Brown et al. 1997, DiCenso et al. 1994, Eggers et al. 1996, Hu et al. 1996, Kruger et al. 1996, and Simpson et al. 1996).

D2.0 COMPARISON OF COMPONENT INVENTORY VALUES

The non radioactive and radioactive HDW model inventories for tank 241-S-103 are listed in Tables D2-1 and D2-2. Table D2-1 lists nonradioactive components on a kilogram (kg) basis, and Table D2-2 lists the radioactive components on a curie basis. The tank volume used to generate the inventories is 938.7 kL (248 kgal) total waste. Hanlon (1996) reports 938.7 kL (248 kgal) total waste, with a sludge layer of 37.8 kL (10 kgal), 836.5 kL (221 kgal) of salt cake, and 64.3 kL (17 kgal) supernatant. Agnew et al. (1996) in the HDW model reports the same 938.7 kL (248 kgal) of total waste, 34.1 kL (9 kgal) of R sludge, 389.9 kL (103 kgal) of SMMS2 salt cake, 450.4 kL (119 kgal) of SMMS1 salt cake, and 64.3 kL (17 kgal) of supernatant. The mean sludge density, including interstitial liquid, used to calculate the engineering estimate component inventories (from similar tanks) was 1.77 g/mL for sludge, 1.63 g/mL for SMMS1 salt cake, and 1.56 g/mL for SMMS2 salt cake. The mean density used for the HDW model density for the total solid waste is 1.59 g/mL.

HDW model density for the total solid waste is 1.59 g/mL. (The chemical species are reported without charge designation per the best-basis inventory convention.)

Table D2-1. Hanford Defined Waste Model-Based Inventory Estimates for Nonradioactive Components in Tank 241-S-103.

Analyte[a]	HDW[b] inventory estimate (kg)	Analyte	HDW[b] inventory estimate (kg)
Al	45,100	OH	123,000
Bi	283	oxalate	3.34
Ca	1,650	Pb	199
Cl	7,200	P as PO_4	8,640
Cr	4,510	Si	2,190
F	1,450	S as SO_4	23,000
Fe	2,340	Sr	1.30
K	2,150	TIC as CO_3	26,400
La	6.16	TOC	12,500
Mn	212	U_{TOTAL}	3,060
Na	264,000	Zr	85.3
Ni	475	H_2O (Wt%)	34.6
NO_2	108,000	density (kg/L)	1.59
NO_3	319,000		

HDW = Hanford Defined Waste
[a] No sample-based data
[b] Agnew et al. (1996).

Table D2-2. Hanford Defined Waste Model-Based Inventory Estimates for Selected Radioactive Components in Tank 241-S-103.

Analyte[a]	HDW[b] inventory estimate (Ci)
^{90}Sr	153,000
^{137}Cs	249,000
$^{239/240}Pu$	81

HDW = Hanford Defined Waste
[a] No sample-based data
[b] Agnew et al. (1996) radionuclides 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 influence the HDW model component inventories.

Tank 241-S-103 was filled with waste from the REDOX facility from the fourth quarter of 1953 until the fourth quarter of 1973. Tank 241-S-103 received a small amount (about 162.8 kL [43 kgal]) of a waste water early in 1955. Later in 1955, the tank received R waste from 241-S-106. Anderson (1990) and Agnew et al. (1995) both have little information about this tank. From the fourth quarter of 1973 until the second quarter of 1976, the tank received bottoms and recycle streams from the 242-S Evaporator/Crystallizer. In the fourth quarter of 1976, the tank became a low-heat evaporator dump tank containing evaporator feed waste. Between the second quarter of 1978 and the fourth quarter of 1980, the tank was classified as having non-complexed, partial neutralized feed and double-shell slurry feed wastes.

The tank was removed from service in 1980 and was partially isolated in December 1982. A jet pump was installed in 1978. New tank photos were taken in 1978 and 1979. The tank level was adjusted in November 1978, October 1979, and November 1980.

D3.1 EXPECTED TYPE OF WASTE BASED ON THIS EVALUATION

Agnew et al. (1996): R, SMMS1, SMMS2
Hill et al. (1995): R, EB, DSSF

R	=	high-level REDOX waste
SMMS1	=	Supernatant Mixing Model S, (early period), a mixture of supernatant coming from the 242-S Evaporator that are a blend of other waste types, that upon cooling precipitated as a salt cake
SMMS2	=	Supernatant Mixing Model S (later period), a mixture of supernatant coming from the 242-S Evaporator that are a blend of other waste types, that upon cooling precipitated as a salt cake
EB	=	evaporator bottoms (same as salt cake)
DSSF	=	Double-shell slurry feed (more selectively concentrated EB)

Agnew et al. (1996) provides estimated volumes for these waste types, as does Hanlon (1996), and these are addressed in Section D2.0. Agnew et al. projects essentially the same total volumes as does Hanlon. The only difference is that Hanlon reports 3.78 kL (1 kgal) more sludge and 3.78 kL (1 kgal) less salt cake than does Agnew et al. Since there are no sample-based inventories and the engineering assessment-based inventories will be compared to the HDW model-based inventories, Agnew's volume estimates will be used. Again, the difference between Hanlon and Agnew is too small to make any significant difference.

D3.2 ASSUMPTIONS USED

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

- Tank waste mass is calculated using the measured average density of similar tanks and the total tank volume listed in Hanlon (1996) and Agnew et al. (1996). The Agnew et al. salt cake and sludge volumes are used as explained in Section D2.0.

- Only the SMMS1 and SMMS2 salt cake waste streams and the R sludge waste streams contributed to solids formation.

- The salt cake and sludge can be estimated by using sample-based concentrations or inventories from similar wastes for calculating the tank 241-S-103 inventory. The supernatant is estimated in this case by volume ratio against the measured supernatant from tank 241-S-101. Tank 241-S-102 is the other tank in the same cascade as tanks 241-S-101 and 241-S-103, and tank 241-S-102 does not have a supernatant layer.

- No radiolysis of NO_3 to NO_2 and no additions of NO_2 to the waste for corrosion purposes are factored into this evaluation.

D3.3 BASIS FOR CALCULATIONS USED IN THIS ENGINEERING EVALUATION

Table D3-1 shows the engineering evaluation approaches used on tank 241-S-103.

Table D3-1. Engineering Evaluation Approaches Used On 241-S-103.

Type of Waste	How Calculated	Check Method
Supernatant Volume = 64.3 kL (17 kgal)	Based on a simple volume ratio with tank 241-S-101. The supernatant from 241-S-101 was measured and represented 45.4 kL (12 kgal) of liquid. Tank 241-S-103 is reported to contain 64.3 kL (17 kgal) of supernatant. Therefore the supernatant inventories for tank 241-S-101 were multiplied by 17/12 = 1.4167 to obtain the 241-S-103 engineering assessment-based inventories for supernatant. See Table D3-5.	None available. It is noted that supernatants from tank to tank are quite variable and this is the best estimate for this supernatant, but may not be very reliable. This portion of the waste contributes very little to the total inventory.
Salt Cake Engineering Assessment SMMS1 Volume = 450.4 kL (119 kgal) Density = 1.63 g/mL (average of 241-S-101, 241-S-102, 241-U-106, and 241-U-109 tank densities) SMMS2 Volume = 389.9 kL (103 kgal) Density = 1.56 g/mL (average of 241-S-101, 241-S-102, 241-U-102, 241-U-107, and 241-U-109 tank densities)	Sample concentrations from other TCR Based tanks with SMMS1 and SMMS2 salt cake were used to predict the salt cake inventories. Waste records for tank 241-S-103 indicate that the salt cake in this tank should be similar to those used to predict the inventories. The calculations are explained just before and within Tables D3-2 and D3-3.	Since there is no sample-based inventory, none was used.
Sludge Engineering Assessment R (assumed for all sludge) Volume = 34.1 kL (9 kgal) Density = 1.773 (average of 241-S-104, 241-S-107, and 241-S-101 tank densities)	Sample concentrations from other TCR Based tanks with R sludge were used to predict the sludge inventories. Waste records for tank 241-S-103 indicate that the sludge in this tank should be similar to those used to predict the inventories. The calculations are explained just before and within Tables D3-4 and D3-6.	Since there is no sample-based inventory, none was used.

D3.3.1 Basis for Salt Cake Calculations Used in this Engineering Evaluation

Sample concentrations from other tanks with SMMS1 and SMMS2 salt cakes were used to predict the salt cake inventories for tank 241-S-103. Waste records for tank 241-S-103 indicate that the salt cake in this tank should be similar to those used to predict the inventories. See Tables D3-2 and D3-3 for calculations and Table D3-6 for summations for total engineering assessment-based inventories. Calculations are: (average concentration of analyte in μg/g) x (waste in kgal) x 3,785 L/kgal x 1,000 mL/L x (density in g/mL) x kg/(1 E+09) μg = total kg for this waste type in the tank.

Table D3-2. SMMS1 Salt Cake Inventory for Tank 241-S-103 (Based on Average From All Tanks with Tank Characterization Reports). (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 concen-tration[e] (μg/g)	HDW model SMM concentration[f] (μg/g)	241-S-103 SMMS1 inventory[g] (kg)
Al	18,000	15,085	13,620	13,625	15,100	28,700	11,086
Ag	12	17	16	NR	15	NR	11.0
B	110	75	80	NR	88	NR	65
Bi	71	76	<DL	<DL	73.5	197	54
Ca	273	237	336	<DL	282	941	54
Cl	4,500	4,099	2,926	NR	3,842	4,980	2,820
Cr	10,000	4,359	3,170	4,233	5,440	2,060	3,994
F	500	13,596	4,669	NR	6,255	1,010	4,520
Fe	508	1,298	3,096	<DL	1,630	288	1,197
K	1,109	898	1,309	NR	1,110	1,490	815
La	<DL	37	43	NR	40	4.29	29.4
Mn	266	597	1,189	<DL	684	147	502
Na	150,000	189,500	170,500	218,300	182,000	182,000	133,620
Ni	114	49	304	<DL	155	260	114
NO_2	91,000	40,100	56,000	42,900	57,500	73,000	42,216
NO_3	110,000	99,200	147,200	297,000	163,000	222,000	73,000
Pb	91	137	348	NR	192	138	141
PO_4	9,500	114,500	5,888	5,970	34,000	6,010	24,936
P	2,290	33,900	1,949	<DL	12,700	NR	9,324

Table D3-2. SMMS1 Salt Cake Inventory for Tank 241-S-103 (Based on Average From All Tanks with Tank Characterization Reports). (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 concentration[e] (μg/g)	HDW model SMM concentration[f] (μg/g)	241-S-103 SMMS1 inventory[g] (kg)
S	5,940	2,683	3,878	NR	4,170	NR	3,059
Si	5,269	517	176	<DL	1,990	1,510	1,459
SO_4	20,700	12,500	10,774	11,100	13,800	16,000	10,108
Sr	7	<DL	<DL	NR	7	0.901	5.13
TOC	1,900	5,340	24,626	3,920	8,950	8,670	6,568
U	560	1,403	781	<DL	914	2,010	671
Zn	30	32	54	<DL	39	NR	28.3
Zr	14	39	88	NR	47	59.3	34.4
Oxalate	15,400	15,700	9,880	NR	13,700	2.32	10,023
Radionuclides[h] (μCi/g)							Ci
^{90}Sr	252	23	77	9	90	81.8	66,000
^{137}Cs	175	121	175	142	153	171	112,000
Density (g/mL)	1.58	1.69	1.57	1.67	1.63	0	1.63

<DL = Less than the detectable limit.
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) for tank 241-S-103
[g] Based on average density of 1.63 g/mL
[h] Radionuclides are reported as of the sample analysis date.

Calculations for Table D3-3 are: (average concentration of analyte in $\mu g/g$) x (waste in kgal) x 3785 L/kgal x 1,000 mL/L x (density in g/mL) x kg/(1 E+09) μg = total kg for this waste type in the tank.

Table D3-3. SMMS2 Salt Cake Inventory (Based on Average For tank 241-S-103 and All Tanks With Tank Characterization Reports). (2 Sheets)

Analyte	Segments 10-2U[a] 241-S-101 ($\mu g/g$)	Segments 2U-5L[b] 241-S-102 ($\mu g/g$)	Segments 2U[c] 241-S-102 ($\mu g/g$)	Segments 2U-6L[d] 241-S-107 ($\mu g/g$)	Segments 1L-9U[e] 241-S-109 ($\mu g/g$)	Average[f] ($\mu g/g$)	SMMS2 Salt Cake Inventory for tank 241-S-103[h] (kg)
Al	16,925	7,450	10,505	10,612	9,487	10,996	6,687
Ag	12	17	13	16	NR	14	8.8
B	111	58	67	89	NR	81	49
Bi	51	<DL	<DL	270	<DL	161	98
Ca	274	233	310	298	<DL	279	170
Cl	4,607	2,981	4,550	2,515	3,560	3,643	2,216
Cd	8	4	6	8	NR	7	4.0
Cr	8,163	1,577	2,417	2,570	2,570	3,459	2,104
Cu	7	NR	12	10	NR	10	6.0
F	638	267	896	501	299	520	316
Fe	453	65	565	767	1,630	696	423
K	1,225	748	1,360	914	NR	1,062	646
Mg	NR	NR	NR	131	NR	131	79.7
Mn	541	26	137	330	<DL	258	157
Mo	43	63	35	39	NR	45	27.3
Na	153,000	207,000	176,000	205,667	237,333	195,800	119,080
Ni	115	19	77	56	<DL	67	41
NO_2	58,150	28,939	36,250	27,600	42,900	38,768	23,597
NO_3	218,500	514,000	293,000	455,333	407,333	377,633	229,667
Pb	66	47	<DL	149	NR	87	53
PO_4	9,230	15,589	19,950	13,509	5,970	12,850	7,785
P	2,333	2,860	6,187	2,580	7,780	4,348	2,644

Table D3-3. SMMS2 Salt Cake Inventory (Based on Average For tank 241-S-103 and All Tanks With Tank Characterization Reports). (2 Sheets)

Analyte	Segments 10-2U[a] 241-S-101 (μg/g)	Segments 2U-5L[b] 241-S-102 (μg/g)	Segments 2U[c] 241-S-102 (μg/g)	Segments 2U-6L[d] 241-S-107 (μg/g)	Segments 1L-9U[e] 241-S-109 (μg/g)	Average[f] (μg/g)	SMMS2 Salt Cake Inventory for tank 241-S-103[h] (kg)
S	4,713	1,325	4,037	1,090	NR	2,791	1,697
Si	<DL	219	148	194	1,220	445	271
SO_4	21,185	8,553	12,785	4,112	11,000	11,527	7,012
Sr	48	<DL	<DL	9	NR	28	17.03
TOC	NR	1,898	6,417	2,414	2,330	3,265	1,985
U	1,497	<DL	<DL	430	<DL	964	586
Zn	33	21	33	29	NR	29	17.7
Zr	13	<DL	<DL	13	NR	13	7.8
Radionuclides[g] (uCi/g)							Ci
^{90}Sr	252	NR	<DL	0.297	4.81	86	52,300
^{137}Cs	160	NR	136.5	62.06	89.1	112	68,100

<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] Radionuclides are reported as of the date of sample analysis
[h] Based on an average density of 1.56 g/mL.

D3.3.2 Basis for Sludge Calculations used In This Engineering Evaluation

Sample concentrations from other TCR Based tanks with R sludge were used to predict the sludge inventories. Waste records for tank 241-S-103 indicate that the sludge in this tank should be similar to those used to predict the inventories. See Table D3-4 and the next paragraph for calculations and Table D3-6 for the total engineering assessment inventories.

Calculations for Table D3-4 are: (average concentration of analyte in μg/g) x (waste in kgal) x 3785 L/kgal x 1,000 mL/L x (density in g/mL) x kg/(1 E+09) μg = total kg for this waste type in the tank.

Table D3-4. Tank 241-S-103 R Sludge Calculations. (2 Sheets)

Analyte	Tanks (segments) (μg/g)			Average concentration[d] (μg/g)	R1 Sludge inventory for tank 241-S-103 9 kgal (kg)
	241-S-104 total solids[b]	241-S-107 7U-8L[c]	241-S-101 5L-8L[a]		
Al	117,000	56,400	127,000	100,000	6,083
Bi	<45.7	NR	<38.8	<42.2	2.6
Ca	247	234	322	268	16.3
Cr	2,350	1,180	2,230	1,920	116.6
Fe	145	1,160	1,960	1,613	98.0
Pb	29.6	33	37	33.2	2.0
Mn	1,150	83	2,750	1,330	80.7
Ni	56	206	90.7	118	7.1
K	300	457	539	432	26.2
Si	1,330	1,060	1,360	1,250	75.9
Na	121,000	60,400	112,000	97,800	5,941
Sr	424	378	456	420	25.5
U	6,690	8,685	7,684	7,690	467
Zr	33.6	131	36	66.9	4.1
Cl	3,200	1,860	2,050	2,370	144
F	145	150	<65.7	<120	7.3
NO_3	191,000	57,600	191,000	122,500	7,442
NO_2	25,900	34,300	31,100	30,433	1,849

Table D3-4. Tank 241-S-103 R Sludge Calculations. (2 Sheets)

Analyte	Tanks (segments) (μg/g)			Average concentration[d] (μg/g)	R1 Sludge inventory for tank 241-S-103 9 kgal (kg)
	241-S-104 total solids[b]	241-S-107 7U-8L[c]	241-S-101 5L-8L[a]		
PO_4	<2,190	1,630	1,360	<1,730	<105
SO_4	2,270	1,300	897	1,489	90.5
TOC	1,730	NR	NR	1,730	105
CO_3	4,140	NR	NR	4,140	252
density	1.64	1.90	1.77	1.77	1.773
Radionuclides	uCi/g	uCi/g	uCi/g	uCi/g	Ci
^{137}Cs	60.5[e]	74[e]	98[e]	77.6[e]	4,729
^{90}Sr	301[e]	276[e]	NR	288[e]	17,504

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] Radionuclides decayed to January 1, 1994.

D3.3.3 Basis for Supernatant Calculations

The supernatant calculations are based on a simple volume ratio with tank 241-S-101. The supernatant from 241-S-101 was measured and represented 45.4 kL (12 kgal) of liquid. Tank 241-S-103 is reported to contain 64.3 kL (17 kgal) of supernatant. Therefore, the supernatant inventories for tank 241-S-101 were multiplied by 17/12 = 1.4167 to obtain the 241-S-103 engineering assessment-based inventories for supernatant. The supernatant values are shown in Table D3-5.

Table D3-5. Tank 241-S-103 Supernatant Calculations. (2 Sheets)

Analyte	241-S-101 supernatant (total inventory) (12 kgal)	241-S-103 17/12 = 1.4167 x S-101 (17 kgal)
Al	1,100	1,558
B	3.2	4.5
Bi	<1.8	<2.6
Ca	<1.8	<2.6
Cr	36.6	51.8
Fe	<0.9	<1.3
Pb	<1.8	<2.6
Mn	<1.8	<2.6
Ni	<0.36	<0.51
P	56.7	80.3
K	106	150
Si	7.38	10.5
Ag	0.689	0.98
Na	9,680	13,713
Sr	<0.18	<0.26
S	83.7	119
U	<9.0	<12.8
Zn	1.29	1.83
Zr	<0.18	<0.26
Cl	335	475
F	<4.77	<6.76
NO_3	8,150	11,546
NO_2	4,230	5,992
PO_4	162	230
SO_4	254	360
Density	1.36	1.36

The total kg of an analyte for each waste type are added in Table D3-6 to produce the total engineering assessment-based inventory for this tank, the total column is rounded to three significant figures.

Table D3-6. Tank 241-S-103 Engineering Assessment Total Inventory Calculations. (2 Sheets)

Element	241-S-103 SC SMMS1 salt cake (kg)	241-S-103 SC SMMS2 salt cake (kg)	241-S-103 SL sludge (kg)	241-S-103 SU supernatant (kg)	Total tank (kg)
Al	11,086	6,687	6,083	1,558	25,400
Bi	54	98	2.6	<2.6	157
B	65	49	2.8	4.5	121
Ca	54	170	16.3	<2.6	243
Chloride	2,820	2,216	144	475	5,660
Cr	3,994	2,104	116.6	51.8	6,270
Fluoride	4,520	316	7.3	<6.76	4,840
Fe	1,197	423	98	<1.3	1,720
Pb	141	53	2.0	<2.6	197
Mn	502	157	80.7	<2.6	741
Ni	114	41	7.1	<0.51	162
NO_3	73,000	229,667	7,442	11,546	322,000
NO_2	42,216	23,597	1,849	5,992	73,700
Oxalate	10,023	3,773	NR	NR	13,800
PO_4	24,936	7,785	<105	230	33,100
P	9,324	2,644	15.4	80.3	12,100
K	815	646	26.2	150	1,640
Si	1,459	271	75.9	10.5	1,820
Ag	11	8.8	0.6	1.0	21.4
Na	133,620	119,080	5,941	13,713	272,000
Sr	5.13	17.03	25.5	<0.26	48
SO_4	10,108	7,012	90.5	360	13,600
S	3,059	1,697	22.4	119	4,900

Table D3-6. Tank 241-S-103 Engineering Assessment Total Inventory Calculations. (2 Sheets)

Element	241-S-103 SC SMMS1 salt cake (kg)	241-S-103 SC SMMS2 salt cake (kg)	241-S-103 SL sludge (kg)	241-S-103 SU supernatant (kg)	Total tank (kg)
TOC	6,568	1,985	105	NR	8,660
TIC as CO_3	NR	NR	252	NR	NR
U	671	586	467	<12.8	1,740
Zn	28.3	17.7	1.4	1.83	49
Zr	34.4	7.8	4.1	<0.26	46
Density (g/mL)	1.63	1.53	1.77	1.36	
Radio-nuclides[a]	Ci	Ci	Ci	Ci	Ci
^{137}Cs	118,204	71,872	4,729	NR	195,000
^{90}Sr	69,800	55,302	17,504	NR	143,000

NR = Not Reported
SC = Salt Cake
SL = Sludge
Su = Supernatant
Solids = All solids, no distinction made from SC or SL
[a] Radionuclides decayed to January 1, 1994.

The engineering assessment-based inventory values and the HDW model values are compared in Table D3-7.

Selected comparisons follow:

Table D3-7. Comparison of Selected Component Inventory Estimates for Tank 241-S-103 Waste. (2 Sheets)

Component	Engineering assessment[a] (kg)	HDW estimated[b] (kg)
Bi	157	283
Ca	243	1,650
Cl	5,660	7,200
K	1,640	2,150

Table D3-7. Comparison of Selected Component Inventory Estimates for Tank 241-S-103 Waste. (2 Sheets)

Component	Engineering assessment[a] (kg)	HDW estimated[b] (kg)
Ni	162	475
NO_2	73,700	108,000
NO_3	322,000	319,000
Mn	741	212
SO_4	13,600	23,000
Cr	6,270	4,510
Pb	197	199
PO_4	33,100	8,640
F	4,840	1,450
Al	25,400	45,100
U	1,740	3,060
Sr	48	1.3
Zn	49	NR
Si	1,820	2,190
Zr	46	85.3
Fe	1,720	2,340
TIC as CO_3	NR	26,400
TOC	8,660	12,500
Na	272,000	264,000
Radionuclides[c]	Ci	Ci
^{90}Sr	143,000	153,000
^{137}Cs	195,000	249,000

HDW = Hanford Defined Waste
NR = Not reported
[a] Table D3-6
[b] Agnew et al. (1996)
[c] Radionuclides decayed to January 1, 1994.

In comparing individual inventories between the engineering assessment-based inventories and the HDW model-based inventories, several considerations must be evaluated. In this tank, three predominate waste types, R, SMMS1 and SMMS2 contributed to solids formation. Having this many waste types makes comparisons more difficult as numerous interactions can cause variances from what would be expected from a single waste type. Agnew et al. (1996) in the HDW model-based inventories does not show separate concentrations for SMMS1 and SMMS2, but rather a summation of both. This makes comparison on the concentration level more difficult.

The actual contributions (volumes) of each of these types is unknown and only estimated. Both the engineering assessment and the HDW model use the same volumes; this makes them easier to compare in this regard. The supernatant is a small contributor to the total inventory. There is no way to accurately predict the supernatant at this time, since there is no sample-based inventory. A reasonable approach to estimate the supernatant was to use the supernatant concentration from the other two tanks (241-S-101 and 241-S-102) in the same cascade with tank 241-S-103. Only tank 241-S-101 had supernatant, and its concentrations were used to predict the supernatant values for this tank (241-S-103). It is recognized that the error in this approach is higher but the inventory is affected only slightly.

The HDW model assumes a less dense solids mass and used one density for the entire solids mass (1.59 g/mL). The engineering assessment is based on actual average sample density measurements from similar tanks for each of the three solid wastes. The engineering assessment densities were R = 1.77 g/mL, SMMS1 = 1.63 g/mL and SMMS2 = 1.56 g/mL. Overall, the density differences are minor and would not cause significant differences in comparative inventories.

At this time, there is no way to accurately predict the salt cake analytical values through an engineering assessment, other than by using analytical data from other tanks containing SMMS1 and SMMS2. The majority of this tank's inventory is from salt cake with small contributions from R sludge and supernatant. Best-basis evaluations dealing with different sludge waste types have shown that the solubilities of some analytes determined from flowsheet and sample data do not agree with the HDW model treatment of solubilities. Solubility assumptions affect the Agnew et al. salt cake predictions because flowsheet analytes not found in the sludge are placed by the HDW model in the salt cakes. This can be true in the reverse case also, in that analytes predicted to remain in the sludge can in reality be carried over into the salt cake. Specific problems cannot be fully isolated at this time, however an attempt is made to discuss the two inventories for this tank.

The inventories for the engineering assessment-based inventory and the HDW model-based inventory were found to be somewhat comparable in the following analytes: Bi, Cl, K, Nitrite, Nitrate, Sulfate, Cr, Pb, Si, Fe, Na, TOC, ^{90}Sr, and ^{137}Cs. Individual discussions will follow about other analytes where larger percentage differences occurred.

Calcium. The engineering assessment-based inventory generally was close to the sample-based inventory for the other two tanks in the cascade (241-S-101 and 241-S-102). The HDW model calcium solubility for salt cake is much lower than in other waste types. This would cause an over-prediction of calcium in the tank by the model.

Nickel. It appears that the higher corrosion source term in the HDW model contributes to its over prediction of nickel in these waste types. The HDW solubility prediction for nickel may not be accurate.

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 manganese was 1,328 μg/g. Interestingly, the HDW SMMS1 slat cake composition estimate for manganese was 684 μg/g, much higher than would be expected based on solubility considerations. It should be noted that there are large ranges in both the SMMS1 and R1 data sets for manganese.

Phosphate. This analyte is quite variable in this cascade. It is very high in 241-S-102, which was a "receiver" tank, and it was about 15 times lower in tank 241-S-101, than in 241-S-102. It is assumed that 241-S-103 would be more similar to 241-S-101 for this analyte, since this tank was not a "receiver" tank. Therefore, the model estimate is being used for this tank.

Fluoride. The fluoride sample-based data for tanks 241-S-101 and 241-S-102 are also quite variable in this cascade. In this tank, the engineering-based inventory is about two and one half times that of the HDW model-based inventory. The engineering assessment-based value is being used as the best basis for tank 241-S-103, but the actual inventory could be between these two values.

Aluminum. The situation with aluminum is similar to that of phosphate and fluoride in this cascade of tanks. The HDW model predicted 50 percent high in 241-S-102 and 50 percent low in 241-S-101. The engineering assessment-based value was used as the best basis.

Uranium. The HDW model inventory for this tank is about 80 percent higher than the engineering assessment-based inventory. Based on volume and waste type comparisons to the other two tanks in cascade with tank 241-S-103, the lower of the two values seems more reasonable.

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. (1996).

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

Information about chemical, radiological, and/or physical properties is used to perform safety analyses, engineering evaluations, and risk assessment associated with waste management activities, as well as regulatory issues. These 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 the waste into a form that is suitable for long-term storage/disposal.

Chemical and radiological inventory information are generally derived using three approaches: (1) component inventories are estimated using results of sample analyses, (2) component inventories are estimated using the HDW Model based on 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. Not surprisingly, the information derived from these different approaches is often inconsistent.

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 chemical information for tank 241-S-103 was performed, including the following:

- An inventory estimate generated by the HDW model (Agnew et al. 1996)
- An engineering evaluation that produced a predicted SMMS1 and SMMS2 salt cake and R sludge inventory based on comparisons developed by evaluation of similar tanks

Based on this evaluation, a best-basis inventory was developed for tank 241-S-103 for which sample information was not available. The engineering assessment-based evaluation inventory was generally chosen as the best basis for those analytes for which sample-based analytical values were available from similar tanks for the following reasons:

- The sample-based inventory analytical concentrations of the other tanks compared favorably with each other for SMMS1 and SMMS2 salt cakes and R sludge

- No methodology is available to fully predict SMMS1 and SMMS2 from process flowsheet or historical records

- The engineering assessment supported the assumption that the sample-based data and engineering assessment-based data from similar tanks appear reasonable

- For those few analytes where poorer agreement was observed between the engineering assessment-based data and the sample-based inventory of the similar tanks, the HDW model values were used.

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 best-basis inventory for tank 241-S-103 is presented in Tables D4-1 and D4-2. and is 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-S-103 (Effective May 31, 1997). (2 Sheets)

Analyte	Total inventory (kg)	Basis (S, M, E, or C)[1]	Comment
Al	25,400	E	
Bi	157	E	
Ca	243	E	
Cl	5,660	E	
TIC as CO_3	26,400	M	No E estimate
Cr	4,510	M	
F	4,840	E	Model 1,450 (May be between these estimates)
Fe	1,720	E	
Hg	1.79	M	No E estimate
K	1,640	E	
La	6.16	M	No E estimate
Mn	741	E	
Na	272,000	E	
Ni	162	E	
NO_2	73,700	E	
NO_3	322,000	E	
OH_{TOTAL}	105,000	C	
Pb	197	E	
P as PO_4	8,640	M	E predicts 33,100 (may be between these two values)
Si	1,820	E	
S as SO_4	13,600	E	
Sr	48	E	
TOC	8,660	E	M Predicts 12,500 (may be between these two values)

Table D4-1. Best-Basis Inventory Estimates for Nonradioactive Components in Tank 241-S-103 (Effective May 31, 1997). (2 Sheets)

Analyte	Total inventory (kg)	Basis (S, M, E, or C)[1]	Comment
U_{TOTAL}	1,740	E	The model predicts 3,060 (may be between these two values)
Zr	46	E	The model predicts 85.3

[1]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_3, NO_2, PO_4, SO_4 and SiO_3.

Table D4-2. Best-Basis Inventory Estimates for Radioactive Components in Tank 241-S-103 Decayed to January 1, 1994 (Effective May 31, 1997). (2 Sheets)

Analyte	Total inventory (Ci)	Basis (S, M, or E)[1]	Comment
^{3}H	254	M	
^{14}C	36.5	M	
^{59}Ni	2.86	M	
^{60}Co	40.4	M	
^{63}Ni	278	M	
^{79}Se	3.64	M	
^{90}Sr	143,000	E	
^{90}Y	143,000	E	Referenced to ^{90}Sr
^{93}Zr	17.8	M	
^{93m}Nb	13.0	M	
^{99}Tc	260	M	
^{106}Ru	0.00717	M	
^{113m}Cd	93.4	M	
^{125}Sb	173	M	
^{126}Sn	5.49	M	
^{129}I	0.501	M	
^{134}Cs	2.74	M	
^{137}Cs	195,000	E	
^{137m}Ba	184,000	E	Referenced to ^{137}Cs
^{151}Sm	12,800	M	
^{152}Eu	4.41	M	
^{154}Eu	655	M	
^{155}Eu	258	M	
^{226}Ra	1.92 E-04	M	
^{227}Ac	0.00114	M	
^{228}Ra	0.151	M	
^{229}Th	0.00354	M	
^{231}Pa	0.00452	M	

Table D4-2. Best-Basis Inventory Estimates for Radioactive Components in Tank 241-S-103 Decayed to January 1, 1994 (Effective May 31, 1997). (2 Sheets)

Analyte	Total inventory (Ci)	Basis (S, M, or E)[1]	Comment
^{232}Th	0.010	M	
^{232}U	0.776	M	
^{233}U	2.97	M	
^{234}U	0.876	M	
^{235}U	0.0356	M	
^{236}U	0.0274	M	
^{237}Np	0.952	M	
^{238}Pu	1.70	M	
^{238}U	1.01	M	
^{239}Pu	66.8	M	
^{240}Pu	10.9	M	
^{241}Am	61.8	M	
^{241}Pu	113	M	
^{242}Cm	0.164	M	
^{242}Pu	6.10 E-04	M	
^{243}Am	0.00214	M	
^{243}Cm	0.0148	M	
^{244}Cm	0.145	M	

[1]S = Sample-based
M = Hanford Defined Waste model-based (Agnew et al. 1996)
E = Engineering assessment-based.

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D5.0 APPENDIX D REFERENCES

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