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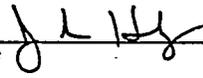
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7. Abstract

Tank 241-TX-118 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. The drivers and objectives of waste tank headspace sampling and analysis are discussed in "Program Plan for the Resolution of Tank Vapor Issues" (Osborne and Huckaby 1994). Tank 241-TX-118 was vapor sampled in accordance with "Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution (Osborne et al., 1994).

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Tank 241-TX-118 Vapor Sampling and Analysis Tank Characterization Report

X.0 INTRODUCTION

Tank TX-118 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). Tank TX-118 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

Tank TX-118 was sampled on September 7, 1994 using the *in situ* sampling (ISS) method (Pingel 1994), and again on December 16, 1994 using the more robust vapor sampling system (VSS), (WHC 1995). Because of changes in laboratory contracts, SUMMA^{TM,1} canister samples from these 2 sampling events were analyzed by different laboratories, using different methods. Results from other samples collected by the ISS method are considered less accurate, because of ISS equipment flow-measuring limitations. Results presented here represent the best available data on the headspace constituents of tank TX-118.

X.1 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank TX-118 using the VSS on December 16, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by *Tank 241-TX-118 Tank Characterization Plan* (the TCP), (Carpenter 1994). The tank headspace temperature was determined to be 21.5 °C. Air from the TX-118 headspace was withdrawn from a single elevation via a 7.9-m long heated sampling probe mounted in riser 9A, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C. All tank air samples were collected between 10:30 a.m. and 2:15 p.m., with no anomalies noted.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), and Pacific Northwest Laboratories (PNL). The 32 tank air samples and 2 ambient air control samples collected during the December sampling event are listed in Table X-1 by analytical laboratory. Table X-1 also lists the 13 trip blanks and 1 field blank provided by the laboratories.

A general description of vapor sampling and sample analysis methods is given by Huckaby (1995). The sampling equipment, sample collection sequence,

¹ SUMMA is a trademark of Molectrics, Inc., Cleveland, Ohio.

sorbent trap sample air flow rates and flow times, chain of custody information, and a discussion of the sampling event itself are given in WHC 1995 and references therein.

X.2 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA™ canister tank air samples for selected inorganic gases and vapors are given in Table X-2 in parts per million by volume (ppmv). Inorganic analyte sorbent traps were prepared and analyzed by PNL (Lucke et al. 1995a).

SUMMA™ samples collected during the ISS event in September 1994 were analyzed by OGIST. SUMMA™ samples collected during the VSS event in December 1994 were analyzed by PNL. Both OGIST and PNL SUMMA™ sample results are listed in Table X-2, with the PNL results placed in brackets. OGIST used different analytical equipment and methods to analyze the carbon dioxide and carbon monoxide, the hydrogen, and the nitrous oxide. This provided low detection limits, and the results, as indicated in the last column of Table X-2, are quite precise. PNL used a single instrument to measure all of the inorganic gases, for which the detection limits were not as low. Reports by PNL (Lucke et al. 1995a) and OGIST (Rasmussen 1994) describe sample preparation and analyses.

X.2.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 33 ppmv, is greater than the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv for ammonia (NIOSH 1995). Ammonia has been observed in virtually all of the waste tanks sampled to date, at concentrations ranging from about 3 ppmv in tank C-108 (Lucke et al. 1995b), to 1040 ppmv in BY-108 (McVeety et al. 1995).

The concentration of hydrogen in tank TX-118 was measured to be 97 ppmv by OGIST, and < 94 ppmv by PNL. Hydrogen in the waste tanks is of concern as a fuel. Given that the lower flammability limit (LFL) for hydrogen in air is about 4 % by volume, the 97 ppmv hydrogen concentration in tank TX-118 corresponds to about 0.24 % of its LFL. At this level, hydrogen is not a flammability concern in tank TX-118.

The nitrous oxide concentration in tank TX-118 was measured to be 17 ppmv by OGIST and 29 ppmv by PNL. These values are about the same as the NIOSH 8-hr REL of 25 ppmv for nitrous oxide (NIOSH 1995). Nitrous oxide, also known as laughing gas, has been detected in other passively ventilated waste tanks at concentrations as low as about 12 ppmv in tank TX-105 (Klinger 1995), and as high as about 800 ppmv in tank C-103 (Huckaby and Story 1994).

X.2.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank TX-118 headspace, measured by OGIS to be 2.5 ppmv in SUMMATM samples, is much higher than in ambient air, where it typically ranges from 0.05 to 0.15 ppmv. Elevated waste tank headspace carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks. Carbon monoxide have not been observed at very high levels in any of the waste tanks, the highest level measured to date was 26.7 ppmv in tank C-103 (Huckaby and Story 1994). The 2.5 ppmv of carbon monoxide in tank TX-118 is much less than the NIOSH 8-hr REL of 35 ppmv.

The carbon dioxide concentration in the tank TX-118 headspace was measured by OGIS to be 54 ppmv, and by PNL to be 98 ppmv. Carbon dioxide is normally present in the ambient air at a concentration of 350 to 400 ppmv, and is typically lower than ambient in the waste tank headspaces. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. Carbon dioxide is neither toxicologically important nor flammable, but because it can be measured at the same time as other gases, and may help characterize the waste, it was listed as a target analyte in the TCP.

X.2.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank TX-118 headspace were determined to be 0.42 ppmv and ≤ 0.03 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank TX-118. The measurable presence of nitric oxide may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. The NIOSH 8-hr REL is 25 ppmv for nitric oxide, and the 15-minute short term exposure limit (STEL) for nitrogen dioxide is 1 ppmv.

The water vapor concentration of tank TX-118 was determined to be about 8.0 mg/L, at the measured tank headspace temperature of 21.5 °C and pressure of 989 mbar (742.1 torr), (WHC 1995). This corresponds to a water vapor partial pressure of 10.8 mbar (8.1 torr), to a dew point of 8.1 °C, and to a relative humidity of 42 %.

Silica gel sorbent traps were used to test for tritium. It is assumed that tritium produced by the waste combines with hydroxide ions to form tritium-substituted water. Evaporation of the tritium-substituted water would then result in airborne radioactive contamination. Silica gel sorbent traps adsorb virtually all (normal and tritium-substituted) water vapor from the sampled tank air, and are analyzed at the WHC 222-S laboratory. Radiochemical analysis of the silica gel trap indicated the total activity of the headspace to be less than 50 pCi/L (WHC 1995).

X.2.4 Discussion of Inorganic Gases and Vapors

Aside from water and carbon dioxide, the most abundant waste constituents in the tank TX-118 headspace are hydrogen, ammonia, and nitrous oxide. These have been detected in most tank headspaces sampled to date, and are usually the dominate waste species.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table X-2 are good, with the exception of the PNL nitrous oxide measurement. Relative standard deviations range from about 1 % for hydrogen to 84 % for the PNL nitrous oxide measurement. The relatively poor precision of the PNL nitrous oxide measurements was apparently due to the fact that they are close to the PNL detection limit. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), the relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

X.3 ORGANIC VAPORS

Organic vapors in the tank TX-118 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Gas chromatography (GC) and mass spectroscopy (MS) were used by both laboratories to separate, identify, and quantitate the analytes. Methane and total nonmethane organic compound (TNMOC) concentrations in SUMMA™ samples from the September 1994 sampling event were measured by OGIST using GC and flame ionization detection (FID). Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995), Rasmussen (1994), and Lucke et al. (1995a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank TX-118. ORNL analyses of TST samples from this and other waste tanks generally agree with, support, and augment the SUMMA™ sample results. However, because certain WHC quality assurance requirements were not satisfied by ORNL, the quality assurance assessment of ORNL by Hendrickson (1995) should be reviewed before results unique to the TST samples are used for decision making.

X.3.1 Positively Identified Organic Compounds

Positive identification of organic analytes using the methods employed by PNL and ORNL involves matching the GC retention times and MS data from a sample with that obtained when known compounds were analyzed. The concentration of an analyte in the sample is said to be quantitatively measured if the response of the GC/MS has been established at several known concentrations of that analyte (i.e., the GC/MS has been calibrated for that analyte), and the MS response to the analyte in the sample is between the lowest and highest responses to the known concentrations (i.e., the analyte is within the calibration range).

ORNL and PNL were assigned different lists of organic compounds, or target analytes, to positively identify and measure quantitatively. The ORNL target analyte list was derived from a review of the tank C-103 headspace constituents by a panel of toxicology experts (Mahlum et al. 1994). The PNL target analyte list was 40 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method list, which consists primarily of halocarbons and common industrial solvents, plus 14 analytes selected from the toxicology panel's review of tank C-103.

Table X-4 lists the organic compounds positively identified and quantitated in SUMMATM samples. Analysis for methane was performed by OGIST (Rasmussen 1994), other SUMMATM analyses were performed according to the Environmental Protection Agency (EPA) task order 14 (TO-14) methodology by PNL (EPA 1988, Lucke et al. 1995a). The quantitation limit for all the target analytes was 0.005 ppmv. Trichlorofluoromethane was the only analyte of the 40 TO-14 target analytes reported to be above the quantitation limit, and only 2 of the 14 additional target analytes were reported to be above the quantitation limit. Averages reported are from analyses of 3 SUMMATM canister samples.

Jenkins et al. (1995) report the positive identification of 25 of 27 target analytes in TST samples. Dibutyl butylphosphonate and tributyl phosphate were the only target analytes not detected in the TST samples. The sampling method is thought to affect these low volatility compounds, however, and their absence in the TST samples does not prove they are not in the tank headspace. 1,1-Dichloroethene was positively identified in 2 of the 3 TSTs analyzed, but its concentration was too low to be quantitatively measured. The average concentrations of the remaining 24 target analytes, from the analysis of 3 TSTs, are given in Table X-4. Despite calibration of the instrument over about a 20-fold concentration range, 5 of the compounds listed in Table X-4 were outside of the calibration range in at least 2 of the samples.

Eleven target analytes were common to both TST and SUMMATM analyses. Table X-5 lists these, and their reported average concentrations in TST and SUMMATM samples. The reported TST sample concentrations of chlorinated compounds (i.e., 1,1-dichloroethene and dichloromethane) and nonpolar compounds (i.e., benzene, toluene, n-hexane, n-heptane, and n-decane) in Table X-5 are all < 0.009 ppmv, and near or below the SUMMATM analysis method detection limit of 0.005 ppmv.

The acetone concentration in the SUMMATM samples was reported to be 2.5 times as high as in TST samples. Comparison of SUMMATM and TST analyses of acetone in other waste tank samples indicates a similar relationship in 7 of the 8 waste tanks reported to date², for which acetone has been quantitatively measured in SUMMATM samples. When compared to the 250 ppmv NIOSH 8-hr REL for

² The acetone concentrations in tanks BY-103, BY-107, BY-110, BY-111, C-103, TX-105, and TX-118 in SUMMATM samples were reported to be 1.7 to 4.5 times higher than in TST samples. In the tank BY-108 samples the same factor was about 0.5.

acetone, even the more conservative value of 1.5 ppmv appears to be insignificant.

There is a similar disagreement regarding nitrile concentrations in SUMMA™ and TST samples from tank TX-118. As shown in Table X-5, the average concentrations of acetonitrile, propanenitrile, and butanenitrile in TST samples were well above the 0.005 ppmv SUMMA™ method detection limit, yet these analytes were not found in the SUMMA™ samples. In lieu of reasons to discount the TST results, they should be used as the best measurement of these nitriles.

X.3.2 Tentatively Identified Organic Compounds

In addition to the target analytes, the ORNL and PNL analytical procedures allow the tentative identification of other organic compounds. Tentative identification of analytes was performed by comparing the MS molecular fragmentation patterns with a library of known MS fragmentation patterns. This method allows an organic analyte to be identified (with reasonable certainty) as an alkane, a ketone, an aldehyde, etc., and may also determine its molecular weight. The method usually does not, however, allow the unambiguous identification of structural isomers, and this ambiguity increases with analyte molecular weight. Many analytes can be tentatively identified with reasonable confidence without having to inject each into the GC/MS to determine their GC retention times or specific MS patterns.

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and SUMMA™ samples. Analyses of the samples are designed to recover, separate, and identify the organic vapors in the samples. TSTs are not good for collecting highly volatile compounds (i.e., molecules more volatile than propane), but are quite good for most others. In contrast, the recovery of very low volatility compounds (i.e., molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (i.e., butanal) from SUMMA™ samples has been problematic.

The list of tentatively identified compounds recovered from SUMMA™ samples, with estimated concentrations, is given in Table X-6. In Table X-6, only non-zero results are included in the reported averages. The list of tentatively identified compounds detected in TST samples, and their estimated concentrations, is given in Table X-7. The averages reported by ORNL in Table X-7 are all 3-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995) and Lucke et al. (1995a), respectively, and should be reviewed before this data is used for decision making. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption

depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

Concentrations given in Tables X-6 and X-7 should be considered rough estimates. Results in Tables X-6 and X-7 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 9 and 10 in Table X-7) or the assignment of the same identity to different peaks (e.g., Cmpd # 71, 78, and 85 in Table X-7). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

X.3.4 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables X-4 through X-7 is to separate them into 2 categories: 1) Organic compounds added to tank TX-118 as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

The first category encompasses all organic compounds that were placed into the tank as waste. It includes the semivolatile branched alkanes and NPHs, which were used as diluents of tributyl phosphate in several processes. It also includes volatile halogenated compounds, such as the trichlorofluoromethane, which may have been used as solvents in various cleaning operations, and which may have been sent to the waste tanks when contaminated. The tentatively identified hexamethylcyclsiloxane (i.e., Cmpd # 45 in Table X-7) is also in this category. Small quantities of siloxanes may have been introduced to the waste tank through their use as process surfactants, but they may also be present in the headspace due to their use in liquid traps at the tank's breather riser.

Two polychlorinated biphenyls (PCBs) were tentatively identified in TST samples from tank TX-118. 3-Chloro-1,1'-biphenyl and 3,3'-dichloro-1,1'-biphenyl (Cmpd # 102 and 104 in Table X-7) were each estimated to be at about 0.005 mg/m³ in the samples, and above the 0.001 mg/m³ NIOSH 8-hr REL recommended for all PCBs. These compounds were used in industry, and presumably at Hanford, in a wide variety of applications as cutting oils, in electrical transformers, lubricants, etc., and their detection in tank TX-118, if valid, could be due to the disposal of small quantities of radiolytically contaminated fluids.

The second category includes all organic compounds that have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables X-3 through X-7 fall into this category, including the alcohols, aldehydes, ketones, nitriles, alkenes, alkyl nitrates, and volatile alkanes, all of which have been associated with the degradation of the NPHs. The hydrolysis of tributyl phosphate, for example, is thought to be the principal source of 1-butanol. By far the most abundant of these in the headspace are the short-chain volatile compounds, however, Table X-7 lists several long-chain low volatility compounds that are also probably waste reaction products.

A large number of nitriles were found in TST samples from TX-118. In addition to the homologous series of straight-chain nitriles from ethanenitrile through decanenitrile, there are also several short unsaturated nitriles and benzonitrile.

Samples from tank TX-118 were found to have a strong signature of organic nitrogen oxides, including alkyl nitrates (i.e., nitric acid esters), alkyl nitrites (i.e., nitrous acid esters), and nitroalkanes. Considering both Tables X-3 and X-6, 5 of the 27 most abundant organic compounds detected in SUMMA™ samples from tank TX-118 are nitrates, and methyl nitrite and nitrosomethane are also amongst the top 27. Such compounds were also detected in TST samples, and they are similarly well represented in Table X-7.

Though it is reasonable to expect alkyl nitrates and nitrites to be produced via chemical and radiolytic processes of the NPHs with other waste, their solubility in the aqueous waste supernate would also be expected to significantly reduce their vapor-phase concentrations. That these constituents are at detectible levels in tank TX-118 may indicate dry conditions where they are formed.

In summary, the organic vapor concentrations in tank TX-118 are relatively low. While not completely typical of NPH-rich tanks, the organic vapors in tank TX-118 clearly indicate the presence of trace amounts of the semivolatiles NPHs and their degradation products. At the reported concentrations, the organic vapors identified in TX-118 do not individually or collectively represent a flammability hazard.

**Table X-1
Tank TX-118 Gas and Vapor Sample Type and Number**

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples				
Oak Ridge National Laboratories	Triple Sorbent Trap	4.0	Organic vapors	4 tank air samples, + 1 trip blanks + 1 field blanks				
				Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blank
								Triethanolamine Sorbent Trap
Pacific Northwest Laboratories	Oxidation Bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blank				
				Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks	
WHC 222-S Laboratory	SUMMA™ canister	6.0	Carbon dioxide, Carbon monoxide, Hydrogen, Nitrous oxide, Organic vapors	3 tank air samples + 2 ambient air samples				
				Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample	

**Table X-2
Tank TX-118 Inorganic Gas and Vapor Concentrations**

Compound	CAS ¹ number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	33	2	6
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	54 [98] ³	0.91 [15]	2 [15]
Carbon Monoxide, CO	630-08-0	SUMMA™	3	2.5 [< 12] ³	0.1 [--]	4 [--]
Hydrogen, H ₂	1333-74-0	SUMMA™	3	97 [< 94] ³	1 [--]	1 [--]
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.42	0.04	10
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.03	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	17 [29] ³	3.5 [24]	20 [84]
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	10,900 (8.0 mg/L)	1,060 (0.8 mg/L)	10

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

3. Unmarked values are from Rasmussen 1994a, values in brackets are from Lucke et al. 1995a.

Table X-3
Tank TX-118 Positively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compound	CAS ¹ Number	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
1	Methane ³	74-82-8	2.4	< 0.06	--
2	Trichlorofluoromethane	75-69-4	0.20	0.01	7
3	2-Butanone	78-93-3	0.027	0.003	10
4	Propanone (acetone)	67-64-1	1.5	0.1	8

1. CAS = Chemical Abstract Service.
2. RSD = relative standard deviation.
3. Methane results are from Rasmussen 1994a.

Table X-4
Tank TX-118 Positively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS ¹ Number	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.046	0.064	139
2	Propanone ³ (acetone)	67-64-1	0.60	0.06	10
3	1,1-Dichloroethene ³ (vinylidene chloride)	75-35-4	< 0.00058	--	--
4	dichloromethane (methylene chloride)	75-09-2	0.0066	0.0079	119
5	Propanenitrile	107-12-0	0.018	0.001	6
6	Butanal ³	123-72-8	0.062	0.034	54
7	n-Hexane	110-54-3	0.0074	0.0023	31
8	Benzene	71-43-2	0.0029	0.0008	29
9	1-Butanol ³	71-36-3	0.27	0.04	15
10	Butanenitrile	109-74-0	0.019	0.005	27
11	2-Pentanone	107-87-9	0.013	0.0001	5
12	n-Heptane	142-82-5	0.0088	0.0004	5
13	Toluene	108-88-3	0.0049	0.0005	9
14	Pentanenitrile	110-59-8	0.0056	0.0012	22
15	2-Hexanone	591-78-6	0.0062	0.0023	37
16	n-Octane	111-65-9	0.0065	0.0022	34
17	Hexanenitrile	628-73-9	0.0026	0.0003	13
18	2-Heptanone	110-43-0	0.0045	0.0017	37
19	n-Nonane	111-84-2	0.0043	0.0013	31
20	Heptanenitrile	629-08-3	0.0026	0.0005	20
21	2-Octanone	111-13-7	0.0011	0.0005	46
22	n-Decane	124-18-5	0.0041	0.0016	38
23	n-Undecane	1120-21-4	0.0027	0.0003	11
24	n-Dodecane	112-40-3	0.0069	0.0022	32
25	n-Tridecane ³	629-50-5	0.021	0.0065	31

Sum of positively identified compounds:	3.4 mg/m ³
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1. CAS = Chemical Abstract Service.
2. RSD = relative standard deviation.
3. Two or more samples were outside calibration range.

Table X-5
Tank TX-118 Comparison of Positively Identified Organic
Compounds in TST and SUMMA™ Samples

Compound	CAS ¹ Number	TST Average (ppmv)	SUMMA™ Average (ppmv)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	< 0.00058	< 0.005
Dichloromethane (methylene chloride)	75-09-2	0.0066	< 0.005
Propanone (acetone)	67-64-1	0.60	1.5
Ethanenitrile (acetonitrile)	75-05-8	0.046	< 0.005
Propanenitrile	107-12-0	0.018	< 0.005
Butanenitrile	109-74-0	0.019	< 0.005
Benzene	71-43-2	0.0029	< 0.005
Toluene	108-88-3	0.0049	< 0.005
n-Hexane	110-54-3	0.0074	< 0.005
n-Heptane	142-82-5	0.0088	< 0.005
n-Decane	124-18-5	0.0041	< 0.005

1. CAS = Chemical Abstract Service.

Table X-6
Tank TX-118 Tentatively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
1	Propene	115-07-1	0.16	0.07
2	Propane	74-98-6	0.58	0.25
3	Methyl nitrite	624-91-9	0.60	0.05
4	Cyclopropane	75-19-4	0.076	0.008
5	Acetaldehyde ²	75-07-0	0.090	0.02
6	Methyl Alcohol	67-56-1	1.6	0.1
7	1-Butene ³	106-98-9	0.057	--
8	Butane	106-97-8	0.13	0.01
9	Nitroso-Methane	865-40-7	0.19	0.02
10	Unknown		0.19	0.06
11	Ethanol	64-17-5	0.18	0.02
12	Isopropyl Alcohol	67-63-0	0.29	0.01
13	Unknown Alkylnitrate		0.18	0.11
14	1-Propanol	71-23-8	0.22	0.02
15	3-Methyl-2-Butanone	563-80-4	< 0.01	--
16	Butanal	123-72-8	0.23	0.01
17	Ethyl nitrate	625-58-1	0.13	0.01
18	Unknown ⁴		0.12	--
19	1-Butanol	71-36-3	0.91	0.02
20	Propyl Nitrate	627-13-4	0.14	< 0.005
21	Butyl nitrate	928-45-0	0.10	0.01
22	3-Heptanone	106-35-4	0.32	0.01
23	Unknown Alkylnitrate		0.091	0.002
Sum of tentatively identified compounds:			6.5	

1. CAS = Chemical Abstract Service.

2. Detected in only 2 samples.

3. Detected in only 1 sample.

4. Detected in only 1 sample.

Table X-7
Tank TX-118 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
1	Methyl nitrite	624-91-9	0.034	0.048
2	1-Propene, 2-methyl-	115-11-7	0.043	0.007
3	Butane	106-97-8	0.034	0.016
4	Methyl Alcohol	67-56-1	0.39	0.10
5	1-Propene, 2-methyl-	115-11-7	0.027	0.023
6	Nitrous acid, butyl ester	544-16-1	0.024	0.0003
7	Methane, dichlorofluoro-	75-43-4	0.0020	0.0030
8	Ethanol	64-17-5	0.18	0.05
9	Trichloromonofluoromethane	75-69-4	0.17	0.02
10	Trichloromonofluoromethane	75-69-4	0.013	0.023
11	Isopropyl Alcohol	67-63-0	0.16	0.02
12	Nitrous acid, butyl ester	544-16-1	0.012	0.001
13	2-Propenenitrile	107-13-1	0.0020	0.0040
14	2-Propanol, 2-methyl-	75-65-0	0.0054	0.0094
15	Nitric acid, ethyl ester	625-58-1	0.037	0.004
16	1-Propanol	71-23-8	0.19	0.04
17	3-Buten-2-one	78-94-4	0.013	0.002
18	2-Butanone	78-93-3	0.087	0.035
19	Nitrous acid, butyl ester	544-16-1	0.028	0.005
20	Nitric acid, propyl ester	627-13-4	0.025	0.005
21	Furan, tetrahydro-	109-99-9	0.024	0.003
22	Butane, 1-chloro	109-69-3	0.0021	0.0037
23	3-Butenenitrile	109-75-1	0.0046	0.0040
24	2-Butenal, (E)-	123-73-9	0.0064	0.0057
25	2-Butanone, 3-methyl	563-80-4	0.0024	0.0042
26	2-Butenenitrile	4786-20-3	0.0071	0.0004
27	3-Pentanone	96-22-0	0.011	0.010

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
28	2-Heptene, (E)-	14686-13-6	0.0047	0.0041
29	1H-Pyrazole, 1-methyl	930-36-9	0.0022	0.0038
30	2-Butanone, 3,3-dimethyl	75-97-8	0.015	0.002
31	2-Heptene, (E)-	14686-13-6	0.0025	0.0043
32	Nitric acid, ethyl ester	625-58-1	0.028	0.006
33	Methyl Isobutyl Ketone	108-10-1	0.0059	0.0053
34	Propanoic acid	79-09-4	0.0046	0.0080
35	Pyrazine	290-37-9	0.0022	0.0038
36	Propane, 2-methyl-2-nitro-	594-70-7	0.018	0.004
37	3-Pentanone, 2-methyl	565-69-5	0.0024	0.0041
38	1-Pentanol	71-41-0	0.022	0.005
39	Octane, 2-chloro-	628-61-5	0.0016	0.0027
40	2-Pentanone, 4,4-dimethyl-	590-50-1	0.020	0.002
41	3-Hexanone	589-38-8	0.0051	0.0013
42	1-Hexanol	111-27-3	0.0049	0.0084
43	2-Furanmethanol, tetrahydro-5-methyl-, trans-	54774-28-6	0.0011	0.0019
44	Tetrachloroethylene	127-18-4	0.011	0.001
45	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0071	0.0062
46	Acetic acid, butyl ester	123-86-4	0.0033	0.0057
47	Nitric acid, butyl ester	928-45-0	0.030	0.014
48	Phenol	108-95-2	0.0021	0.0036
49	Cyclohexane, 1,1-dimethyl	590-66-9	0.0031	0.0027
50	1-Hexanol	111-27-3	0.014	0.0036
51	4-Heptanone	123-19-3	0.011	0.0031
52	Alkenol		0.014	0.002
53	3-Heptanone	106-35-4	0.14	0.04
54	3-Heptanol	589-82-2	0.037	0.012
55	Heptanal	111-71-7	0.0039	0.0033

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Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
56	Cyclopent-2-ene-1-one, 2,3,4-trimethyl	83321-16-8	0.0015	0.0026
57	Cyclobutanone, 3,3-dimethyl	1192-33-2	0.0016	0.0027
58	3-Heptanone, 6-methyl	624-42-0	0.0050	0.0010
59	Nitric acid, pentyl ester	1002-16-0	0.012	0.006
60	2,2'-Bioxepane	74793-02-5	0.0080	0.0071
61	4-Hydroxy-4-methylpentanone		0.018	0.006
62	Pyridine, 2,4-dimethyl-	108-47-4	0.0013	0.0022
63	3-Hepten-2-one, 4-methyl	22319-25-1	0.040	0.016
64	Alkenol		0.018	0.005
65	1-Heptanol	111-70-6	0.023	0.007
66	Cyclohexane, 1-ethyl-4-methyl-, trans	6236-88-0	0.0014	0.0024
67	2,2,4-Trimethyl-3-pentanone	5857-36-3	0.0040	0.0004
68	Octanal	124-13-0	0.0042	0.0036
69	Benzonitrile	100-47-0	0.0020	0.0034
70	Cyclopentane, (2-methylpropyl)-	3788-32-7	0.024	0.012
71	Nitric acid, hexyl ester	20633-11-8	0.0084	0.0073
72	1-Hexanol, 2-ethyl-	104-76-7	0.10	0.05
73	C3-Cyclohexane		0.0050	0.0044
74	Nitric acid, heptyl ester	20633-12-9	0.0032	0.0028
75	1H-Pyrozole, 4,5-dihydro-1, 5-dimethyl- and others		0.010	0.018
76	Alkane		0.024	0.018
77	1-Propanol, 2,2-dimethyl-, nitrate	926-42-1	0.048	0.008
78	Nitric acid, hexyl ester	20633-11-8	0.0042	0.0036
79	1-Octanol	111-87-5	0.021	0.010
80	Heptane, 2,2,4,6,6-pentamethyl-	13475-82-6	0.011	0.008
81	Acetophenone	98-86-2	0.026	0.019

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Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
82	Octanenitrile	124-12-9	0.022	0.015
83	2-Nonanone	821-55-6	0.017	0.021
84	Benzene, nitro-	98-95-3	0.010	0.009
85	Nitric acid, hexyl ester	20633-11-8	0.010	0.009
86	Benzoic acid, 2-[(trimethylsilyl)oxy]-,	3789-85-3	0.0033	0.0028
87	Heptane, 3-ethyl-5-methyl-	52896-90-9	0.0032	0.0028
88	Dodecane, 4-methyl-	6117-97-1	0.0039	0.0034
89	1-Nonanol	143-08-8	0.0071	0.0061
90	Nonanenitrile	2243-27-8	0.0060	0.0052
91	C10-Alkanone		0.0073	0.0064
92	2-Oxazolidinone, 5-methyl-3-(2-propenyl)-	55956-20-2	0.0014	0.0024
93	Nitric acid, decyl ester	2050-78-4	0.0058	0.0051
94	Decane, 2-methyl-	6975-98-0	0.0047	0.0041
95	1-Undecanol	112-42-5	0.0018	0.0031
96	Decanenitrile	1975-78-6	0.0047	0.0040
97	Decane, 5-ethyl-5-methyl-	17312-74-2	0.0066	0.0057
98	Tetradecane	629-59-4	0.020	0.018
99	Biphenyl	92-52-4	0.0029	0.0025
100	Pentadecane	629-62-9	0.0041	0.0036
101	Hexadecanoic acid	57-10-3	0.012	0.020
102	1,1'-Biphenyl, 3-chloro	2051-61-8	0.0047	0.0041
103	Diethyl Phthalate	84-66-2	0.020	0.007
104	1,1'-Biphenyl, 3,3'-dichloro-	2050-67-1	0.0050	0.0044
105	Benzenesulfonamide, N-butyl	3622-84-2	0.036	0.036
106	Isopropyl Palmitate	142-91-6	0.034	0.034
Sum of Tentatively Identified Compounds:			2.6	

1. CAS = Chemical Abstract Service.

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