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TANK 241TX118 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
9/1994 & 12/1994

COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 2

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ECN

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626291

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18. Change Impact Review: Indicate the related documents (other than the engineering documents identified on Side 1) that will be affected by the change described in Block 12. Enter the affected document number in Block 19.

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

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7. Abstract

Significant changes have been made to all of the original vapor characterization reports. This report documents specific headspace gas and vapor characterization results for all vapor sampling events to date. In addition, changes have been made to the original vapor reports to qualify the data based on quality assurance issues associated with the performing laboratories.

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**Tank 241-TX-118 Headspace Gas and Vapor
Characterization Results for Samples
Collected in September 1994 and December 1994**

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**Date Published
September 1995**

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Acronyms and Abbreviations

CES	consensus exposure standard
EPA	Environmental Protection Agency
GC	gas chromatograph
GC/MS	gas chromatograph/mass spectrometer
LFL	lower flammability limit
MS	mass spectrometer
NFPA	National Fire Protection Association
NPH	normal paraffinic hydrocarbon
OGIST	Oregon Graduate Institute of Science and Technology
ORNL	Oak Ridge National Laboratory
PNL	Pacific Northwest Laboratory
ppmv	parts per million by volume, 1 ppmv = 10 ⁻⁴ vol%
TNMOC	total nonmethane organic carbon
TST	triple sorbent trap
vol%	percent by volume, 1 vol% = 10,000 ppmv
VSS	vapor sampling system
WHC	Westinghouse Hanford Company

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**Tank 241-TX-118 Headspace Gas and Vapor Characterization Results
for Samples Collected in September 1994 and December 1994**

1.0 INTRODUCTION

1.1 Characterization Objectives

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). This report primarily discusses results from the December 1994 sampling event, but also includes selected results of the September 1994 sampling event. The tank TX-118 headspace was sampled in September 1994 in accordance with *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991), and in December 1994 in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

1.2 Characterization Data Criteria

Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution describes parameters for data collection to ensure appropriate conclusions can be drawn from the data. Tank headspace characterization data was collected to help in the evaluation of 1) headspace flammability, and 2) identification and quantification of compounds of toxicological concern.

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). Current governing operating specifications for Watchlist tanks, such as tank TX-118, specify that combustible constituents be maintained at or below 20 % of the LFL (WHC 1995a).

Headspace characterization data are used by Westinghouse Hanford Company (WHC) Tank Waste Remediation Systems Industrial Hygiene as source term data in the industrial hygiene strategy to protect workers from tank fugitive emissions. Because selection of worker protective equipment must be based on industrial hygiene monitoring of the work place and not on source term data (29 CFR 1910.120), tank headspace characterization data can not be used for this purpose. Furthermore, because there are mechanisms by which headspace constituents can be either diluted or concentrated as they are released to the atmosphere, the headspace characterization data should not be considered to be representative of emissions at the point of emission.

These statements notwithstanding, the data quality objectives document specifies that the industrial hygiene group be advised if constituents with toxicological properties exceed 50 % of the appropriate consensus exposure standard (CES) for non-carcinogens, or 10 % of the appropriate CES for carcinogens. A CES is defined as the most stringent of known regulatory or recommended toxicological values for the workplace (Osborne et al. 1994).

1.3 Sampling Overview

Tank TX-118 was vapor sampled in September 1994 using the *in situ* sampling (ISS) method, and again in December 1994 using the more robust vapor sampling system (VSS) method. Because the ISS sample volume flow measurement used during the September 1994 event was inherently less accurate than that of the VSS, the sorbent trap samples from the ISS event are not considered to be equivalent to those from the VSS sampling event (Huckaby et al. 1995). Furthermore, there are other discrepancies between results from the ISS and VSS methods that are not understood (Huckaby 1994a), and until the ISS method has been validated and the discrepancies resolved, results from early ISS events should be considered suspect.

Nevertheless, a brief description of the ISS event and hydrogen cyanide sampling results from the September 1994 ISS event are presented below, because this analyte was not sampled for during the VSS event. Huckaby et al. (1995) describe the bases for using the ISS method for hydrogen cyanide, and why it was not sampled for during the VSS event. Also, samples from the September 1994 ISS event were analyzed for total nonmethane organic carbon (TNMOC) by Oregon Graduate Institute of Science and Technology (OGIST), and these results are presented below because this analysis was not performed on samples from the December 1994 VSS sampling event. All other results presented here are from the December 1994 VSS sampling event.

Samples collected are thought to have been representative of the tank headspace when the tank was sampled (Meacham et al. 1995), and sample analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents. No assessment has been made of how the tank TX-118 headspace composition changes with time, though studies of tank C-103 suggest that composition changes probably occur very slowly in passively ventilated tanks, such as tank BY-103 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank TX-118 is the third tank in a 3-tank cascade with tanks TX-116 and TX-117. It is connected to tank TX-117 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade line. Tanks TX-116 and TX-117 are connected by a similar line. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank TX-116 or TX-117 may be transferred to tank TX-118 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data are available for either tanks TX-116 or TX-117 to assess their potential effect on tank TX-118.

The cascade of tanks TX-116, TX-117, and TX-118 is passively ventilated, which means that the tanks are allowed to exhale air, waste gases, and vapors as the barometric pressure falls, and inhale ambient air as the barometric pressure rises. Each of these tanks has its own filtered breather riser. Barometric pressure typically rises and falls on a diurnal cycle, producing an average daily exchange of air equal to about 0.46 % of each tank headspace (Huckaby 1994b). Changes in the concentrations of tank headspace constituents due to barometric pressure changes are consequently very slow.

2.0 SAMPLING EVENT

2.1 September 1994 *In Situ* Sampling Event

Tank TX-118 was sampled using ISS methods on September 7, 1994 by WHC Sampling and Mobile Laboratories. This sampling was conducted to satisfy requirements of *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991). Samples for hydrogen cyanide were collected from a point approximately 7.9 m below the top of the flange on riser 9A, between 11:15 a.m. and 12:15 p.m.

Huckaby et al. (1995) give a general description of the ISS method and equipment. Pingel (1994) provides field sampling information for the tank TX-118 September 1994 ISS event, and Mahon (1995) provides revised sample volume measurements. In addition to the hydrogen cyanide results presented below, Thomas et al. (1995) and Rasmussen (1994) provide sample analysis results.

2.2 December 1994 Vapor Sampling System 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 1995b). 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 2-1 by analytical laboratory. Table 2-1 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 et al. (1995). The sampling equipment, sample collection sequence, 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 (1995b).

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,1} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions as given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM were prepared and analyzed at PNL quality assurance impact level 2 (Lucke et al. 1995a). PNL analyses of SUMMATM canisters and sorbent traps for inorganic compounds were performed 64 and 30 days, respectively, after sample collection (Ligotke 1995). Sorbent trap analyses were within the administratively chosen 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994), but the SUMMATM canister analyses exceeded this. Though no holding time study has been performed to determine the stability of inorganic gases and vapors in SUMMATM canisters in the chemical matrix of the tank samples, these compounds would be expected to be quite stable, and exceeding the holding may not have affected the results.

Analyses of the hydrogen cyanide sorbent traps collected in September 1994 were performed within 9 days of sample collection. Sample preparation and analyses were conducted at PNL quality assurance impact level 3 (Thomas et al. 1995).

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Ammonia concentration in the headspace of tank TX-118 was measured at 33 ppmv. 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). Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 33 ppmv corresponds to about 0.02 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank TX-118 was measured to be < 94 ppmv by PNL. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, the upper bound of 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 29 ppmv by PNL. Nitrous oxide has been detected in other passively ventilated waste tanks at concentrations as low as about 12 ppmv in tank TX-105 (Klinger et al. 1995), and as high as about 868 ppmv in tank U-103 (Ligotke et al. 1995). Under the proper conditions, nitrous oxide can serve as an oxidizer to support combustion. However, Cashdollar et al. (1992) found that nitrous oxide had no significant effect on the flammability of hydrogen and air mixtures for hydrogen concentrations less than 20 vol%, and that "small amounts of nitrous oxide (relative to air) do not appear to have much effect on the flammability". Their results suggest the measured nitrous oxide concentration is much too low to have a significant effect on the flammability of the tank TX-118 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide was determined to be < 12 ppmv in each of the 3 SUMMATM canister samples. Carbon monoxide in ambient air 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

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

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-103² (Huckaby and Story 1994).

The carbon dioxide concentration in the tank TX-118 headspace was measured 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 has been an inorganic target analyte.

3.3 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 $\pm$ 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. These constituents could potentially serve as oxidizers to support combustion, but at the measured concentrations would have a negligible effect on the flammability of the tank TX-118 headspace.

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 1995b). 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 1995b).

3.4 Hydrogen Cyanide

Analysis of the hydrogen cyanide specific sorbent traps indicated the concentration of this analyte to below 0.02 ppmv in all 3 samples (Thomas et al. 1995). The absence of hydrogen cyanide at measurable concentrations is consistent with the expectation that an acid gas, such as hydrogen cyanide, would not exist at significant concentrations above the caustic waste in tank TX-118. No hydrogen cyanide has been detected in any of the 10 waste tank headspaces sampled for this analyte.

3.5 Discussion of Inorganic Gases and Vapors

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

² The carbon monoxide measurement in tank C-103 was made by Oregon Graduate Institute of Science and Technology, and placed in brackets to emphasize it should be considered secondary data.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are good, with the exception of the 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.

4.0 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. Both PNL and ORNL used a gas chromatograph (GC) equipped with a mass spectrometer (MS) detector to separate, identify, and quantitate the analytes. OGIST analyzed 3 SUMMA™ canister samples from the September 1994 sampling event for total nonmethane organic carbon (TNMOC) using the EPA task order 12 (TO-12) method (EPA 1988). Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a), Rasmussen (1994), and Lucke et al. (1995a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank TX-118. PNL results were produced at PNL quality assurance impact level 2. All PNL analyses were completed 92 days after sample collection, and exceeded the WHC quality assurance project plan 60-day holding time (Keller 1994). The 60-day holding time was administratively chosen, because no holding time study has been performed to determine the stability of analytes in SUMMA™ canisters in the chemical matrix of the tank samples.

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.

All TSTs prepared by ORNL had 3 surrogate compounds added to evaluate sample matrix effects, potential handling, storage, and shipment problems, and analytical instrumentation performance (Jenkins et al. 1995a). ORNL evaluated the surrogate recoveries using a statistical approach similar to that prescribed by *SW 846 Method 8260A Volatile Organic Compounds by Gas Chromatography/Mass Spectrometry (GC/MS) Capillary Column Technique* (EPA 1992). Using this approach, ORNL reported that all surrogates had standard deviation values within the 95 % confidence interval for variance, indicating that no bias was introduced in the measurement of analyte quantities (Jenkins 1995a).

4.1 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 4-1 lists the organic compounds positively identified and quantitated in SUMMA™ samples. Analyses for methane were performed with the inorganic gas analyses, other SUMMA™ 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 SUMMA™ canister samples.

Jenkins et al. (1995a) 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 15 quantitated analytes, from the analysis of 3 TSTs, are given in Table 4-2. Table 4-3 lists 5 positively identified compounds that were not quantitated because their measurement in at least 1 TST sample was outside the instrument calibration range. Table 4-4 lists the 5 remaining compounds for which the analyte-specific ORNL practical holding time was exceeded. Data in Table 4-3 should not be considered quantitative, and data in Tables 4-3 and 4-4 may not be accurate to within $\pm 30\%$ as specified by Burnum (1995).

The ORNL practical holding time is defined as the holding time for which there is a 15 % risk that the concentration of an analyte in the sample will be below its initial concentration. As indicated in Table 4-4, propanone, butanal, 1-butanol, 2-pentanone, and n-pentanenitrile exceeded their practical holding times, and may have been affected by the 58 day period between sample collection and analysis (Jenkins 1995b). Jenkins et al (1995b) describe the ORNL practical holding time study, and report practical holding times for these compounds. It should be noted that the contractual holding time for the TST samples was 60 days.

Eleven target analytes were common to both TST and SUMMA™ analyses. Table 4-5 lists these, and their reported average concentrations in TST and SUMMA™ 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 4-5 are all < 0.009 ppmv, and near or below the SUMMA™ analysis method detection limit of 0.005 ppmv.

The propanone concentration in the SUMMA™ samples was reported to be 2.5 times as high as in TST samples. There is a similar disagreement regarding nitrile concentrations in SUMMA™ and TST samples from tank TX-118. As shown in Table 4-4, the average concentrations of ethanenitrile, propanenitrile, and n-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.

4.2 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. Using this method, 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 4-6. In Table 4-6, 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 4-7. The averages reported by ORNL in Table 4-7 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.

Because the list of tentatively identified organic compounds in TST samples is long and locating any given compound may be difficult, the list has been sorted alphanumerically by compound name in Table 4-8, and also in order of decreasing estimated concentrations in Table 4-9. Numbers in the first columns of Tables 4-8 and 4-9 (Cmpd #) identify the location of the compound in Table 4-7.

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 4-6 through 4-9 should be considered rough estimates. Results in Tables 4-6 through 4-9 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 4-7) or the assignment of the same identity to different peaks (e.g., Cmpd # 71, 78, and 85 in Table 4-7). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

4.3 Total Nonmethane Organic Carbon

OGIST measured the TNMOC concentration in 3 SUMMA™ canister samples from the September 1994 ISS event using the EPA TO-12 method (Rasmussen 1994). The sample mean was [9.2 mg/m³], with a standard deviation of [0.4 mg/m³]. This value is about average for other passively ventilated tanks that have been sampled. Because OGIST did not have a WHC-approved quality assurance project plan in place at the time of analyses, OGIST data should be considered secondary data.

4.4 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables 4-1 through 4-7 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 hexamethylcyclotrisiloxane (i.e., Cmpd # 45 in Table 4-7) 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 4-7) were each estimated to be at about 0.005 mg/m³ in the samples. 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 4-1 through 4-7 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 4-7 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 tank 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 4-1 and 4-6, 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 4-9.

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 semivolatile 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.

5.0 SUMMARY

The tank TX-118 headspace was sampled in September 1994 and again in December 1994 for gases and vapors to address flammability and industrial hygiene concerns. Collection and analysis of samples has been reported. It was determined that no headspace constituents exceeded the flammability or industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995b).

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Table 2-1
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
	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blank
Pacific Northwest Laboratories	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blank
	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
	SUMMA™ canister	6.0	Carbon dioxide, Carbon monoxide, Hydrogen, Nitrous oxide, Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
Tank TX-118 Inorganic Gas and Vapor Concentrations --
Analyses Conducted by Pacific Northwest Laboratory

Compound	CAS ¹ number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation ² (ppmv)	RSD ^{2,2} (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	33	2	6
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	98	15	15
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	< 12	—	—
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	< 94	—	—
Hydrogen Cyanide ³ , HCN	74-90-8	Sorbent Trap	3	< 0.02	—	—
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 TM	3	29	24	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. Burnum (1995) specifies the RSD should be less than 25 %.

³ Results for hydrogen cyanide are from the September 1994 ISS event.

Table 4-1
Tank TX-118 Quantitatively Measured Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (ppmv)	Standard Deviation (ppmv)	RSD ³ (%)
1	Methane ⁴	74-82-8	< xxx	—	—
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 Average of 3 samples.

3 RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

4 Methane analyses were performed with analyses of the inorganic gases by PNL.

Table 4-2
Tank TX-118 Quantitatively Measured Organic Compounds in TST Samples –
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Propanenitrile	107-12-0	0.018	0.001	6
2	n-Hexane	110-54-3	0.0074	0.0023	31
3	Benzene	71-43-2	0.0029	0.0008	29
4	n-Butanenitrile	109-74-0	0.019	0.005	27
5	n-Heptane	142-82-5	0.0088	0.0004	5
6	Toluene	108-88-3	0.0049	0.0005	9
7	2-Hexanone	591-78-6	0.0062	0.0023	37
8	n-Octane	111-65-9	0.0065	0.0022	34
9	n-Hexanenitrile	628-73-9	0.0026	0.0003	13
10	2-Heptanone	110-43-0	0.0045	0.0017	37
11	n-Nonane	111-84-2	0.0043	0.0013	31
12	n-Heptanenitrile	629-08-3	0.0026	0.0005	20
13	n-Decane	124-18-5	0.0041	0.0016	38
14	n-Undecane	1120-21-4	0.0027	0.0003	11
15	n-Dodecane	112-40-3	0.0069	0.0022	32

1 Results in this table are quantitative (as defined in Section 4.1).

2 CAS = Chemical Abstract Service.

3 Average of 3, 4-L TST samples.

4 RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

Table 4-3
Tank TX-118 Positively Identified Organic Compounds in TST Samples --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.046	0.064	139
2	1,1-Dichloroethene (vinylidene chloride)	75-35-4	< 0.00058	—	—
3	Dichloromethane (methylene chloride)	75-09-2	0.0066	0.0079	119
4	2-Octanone	111-13-7	0.0011	0.0005	46
5	n-Tridecane	629-50-5	0.021	0.0065	31

1 Results in this table are not quantitative (as defined in Section 4.1) because measured values in at least 1 of the samples are outside instrument calibration limits.

2 CAS = Chemical Abstract Service.

3 Average of 3, 4-L TST samples.

4 RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

Table 4-4
Tank TX-118 Positively Identified Compounds in TST Samples
for which Practical Holding Times were Exceeded --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Propanone ⁵ (acetone)	67-64-1	0.60	0.06	10
2	Butanal ⁶	123-72-8	0.062	0.034	54
3	1-Butanol ⁶	71-36-3	0.27	0.04	15
4	2-Pentanone ⁶	107-87-9	0.013	0.0001	5
5	n-Pentanenitrile ⁶	110-59-8	0.0056	0.0012	22

1 Practical holding times are defined and discussed in Section 4.1.

2 CAS = Chemical Abstract Service.

3 Average of 3, 4-L TST samples.

4 RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

5 The concentration of this analyte was not quantitatively measured (as defined in Section 4.1), because the measured concentration was outside of the instrumental calibration limits.

6 The concentration of this analyte is quantitatively measured (as defined in Section 4.1).

Table 4-5
Tank TX-118 Comparison of Organic Compounds in TST and SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory
and Oak Ridge National Laboratory

Compound	CAS ¹ Number	TST Average ² (ppmv)	SUMMA™ Average ³ (ppmv)	PRD ⁴ (%)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	< 0.00058	< 0.005	—
Dichloromethane (methylene chloride)	75-09-2	0.0066	< 0.005	> 28
Propanone (acetone)	67-64-1	0.60	1.5	86
Ethanenitrile (acetonitrile)	75-05-8	0.046	< 0.005	> 161
Propanenitrile	107-12-0	0.018	< 0.005	> 113
n-Butanenitrile	109-74-0	0.019	< 0.005	> 117
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	> 39
n-Heptane	142-82-5	0.0088	< 0.005	> 55
n-Decane	124-18-5	0.0041	< 0.005	—

1 CAS = Chemical Abstract Service.

2 Average of 3, 4-L TST samples by ORNL.

3 Average of 3 sample analyses by PNL.

4 PRD = percent relative difference. Keller (1994) requires the PRD to be less than 20 %.

Table 4-6
Tank TX-118 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses Conducted by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard ³ 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 ⁴	75-07-0	0.090	0.02
6	Methyl Alcohol	67-56-1	1.6	0.1
7	1-Butene ⁵	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 ⁵		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 Average of 3 samples, values listed are estimates.

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3 When the analyte was detected in only 2 samples, the entry is the relative difference (i.e., their difference divided by 2).

4 Detected in only 2 samples.

5 Detected in only 1 sample.

Table 4-7
Tank TX-118 Tentatively Identified Organic Compounds in TST Samples
in Order of Chromatographic Elution --
Analyses Conducted by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (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

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Cmpd #	Compound	CAS ¹ Number	Average ² (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

Cmpd #	Compound	CAS ¹ Number	Average ² (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
82	Octanenitrile	124-12-9	0.022	0.015
83	2-Nonanone	821-55-6	0.017	0.021

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
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]-, trimethylsilyl ester	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.

2 Average of 3, 4-L TST samples, values listed are estimates.

Table 4-8
 Tank TX-118 Tentatively Identified Organic Compounds in TST Samples
 Sorted Alphanumerically --
 Analyses Conducted by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
77	1-Propanol, 2,2-dimethyl-, nitrate	926-42-1	0.048	0.008
2	1-Propene, 2-methyl-	115-11-7	0.043	0.007
38	1-Pentanol	71-41-0	0.022	0.005
50	1-Hexanol	111-27-3	0.014	0.0036
5	1-Propene, 2-methyl-	115-11-7	0.027	0.023
16	1-Propanol	71-23-8	0.19	0.04
42	1-Hexanol	111-27-3	0.0049	0.0084
79	1-Octanol	111-87-5	0.021	0.010
65	1-Heptanol	111-70-6	0.023	0.007
72	1-Hexanol, 2-ethyl-	104-76-7	0.10	0.05
95	1-Undecanol	112-42-5	0.0018	0.0031
89	1-Nonanol	143-08-8	0.0071	0.0061
102	1,1'-Biphenyl, 3-chloro-	2051-61-8	0.0047	0.0041
104	1,1'-Biphenyl, 3,3'-dichloro-	2050-67-1	0.0050	0.0044
75	1H-Pyrozole, 4,5-dihydro-1, 5-dimethyl- and others		0.010	0.018
29	1H-Pyrazole, 1-methyl-	930-36-9	0.0022	0.0038
92	2-Oxazolidinone, 5-methyl-3-(2-propenyl)-	55956-20-2	0.0014	0.0024
18	2-Butanone	78-93-3	0.087	0.035
40	2-Pentanone, 4,4-dimethyl-	590-50-1	0.020	0.002
83	2-Nonanone	821-55-6	0.017	0.021
14	2-Propanol, 2-methyl-	75-65-0	0.0054	0.0094
13	2-Propenenitrile	107-13-1	0.0020	0.0040
43	2-Furanmethanol, tetrahydro-5-methyl-, trans-	54774-28-6	0.0011	0.0019
24	2-Butenal, (E)-	123-73-9	0.0064	0.0057
25	2-Butanone, 3-methyl-	563-80-4	0.0024	0.0042

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
26	2-Butenenitrile	4786-20-3	0.0071	0.0004
31	2-Heptene, (E)-	14686-13-6	0.0025	0.0043
28	2-Heptene, (E)-	14686-13-6	0.0047	0.0041
30	2-Butanone, 3,3-dimethyl-	75-97-8	0.015	0.002
60	2,2'-Bioxepane	74793-02-5	0.0080	0.0071
67	2,2,4-Trimethyl-3-pentanone	5857-36-3	0.0040	0.0004
63	3-Hepten-2-one, 4-methyl-	22319-25-1	0.040	0.016
23	3-Butenenitrile	109-75-1	0.0046	0.0040
27	3-Pentanone	96-22-0	0.011	0.010
17	3-Buten-2-one	78-94-4	0.013	0.002
53	3-Heptanone	106-35-4	0.14	0.04
37	3-Pentanone, 2-methyl-	565-69-5	0.0024	0.0041
41	3-Hexanone	589-38-8	0.0051	0.0013
54	3-Heptanol	589-82-2	0.037	0.012
58	3-Heptanone, 6-methyl-	624-42-0	0.0050	0.0010
61	4-Hydroxy-4-methylpentanone		0.018	0.006
51	4-Heptanone	123-19-3	0.011	0.0031
46	Acetic acid, butyl ester	123-86-4	0.0033	0.0057
81	Acetophenone	98-86-2	0.026	0.019
76	Alkane		0.024	0.018
52	Alkenol		0.014	0.002
64	Alkenol		0.018	0.005
84	Benzene, nitro-	98-95-3	0.010	0.009
105	Benzenesulfonamide, N-butyl-	3622-84-2	0.036	0.036
86	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.0033	0.0028
69	Benzonitrile	100-47-0	0.0020	0.0034
99	Biphenyl	92-52-4	0.0029	0.0025
3	Butane	106-97-8	0.034	0.016

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
22	Butane, 1-chloro-	109-69-3	0.0021	0.0037
91	C10-Alkanone		0.0073	0.0064
73	C3-Cyclohexane		0.0050	0.0044
57	Cyclobutanone, 3,3-dimethyl-	1192-33-2	0.0016	0.0027
49	Cyclohexane, 1,1-dimethyl-	590-66-9	0.0031	0.0027
66	Cyclohexane, 1-ethyl-4-methyl-, trans-	6236-88-0	0.0014	0.0024
56	Cyclopent-2-ene-1-one, 2,3,4-trimethyl-	83321-16-8	0.0015	0.0026
70	Cyclopentane, (2-methylpropyl)-	3788-32-7	0.024	0.012
45	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0071	0.0062
94	Decane, 2-methyl-	6975-98-0	0.0047	0.0041
97	Decane, 5-ethyl-5-methyl-	17312-74-2	0.0066	0.0057
96	Decanenitrile	1975-78-6	0.0047	0.0040
103	Diethyl Phthalate	84-66-2	0.020	0.007
88	Dodecane, 4-methyl-	6117-97-1	0.0039	0.0034
8	Ethanol	64-17-5	0.18	0.05
21	Furan, tetrahydro-	109-99-9	0.024	0.003
55	Heptanal	111-71-7	0.0039	0.0033
80	Heptane, 2,2,4,6,6-pentamethyl-	13475-82-6	0.011	0.008
87	Heptane, 3-ethyl-5-methyl-	52896-90-9	0.0032	0.0028
101	Hexadecanoic acid	57-10-3	0.012	0.020
11	Isopropyl Alcohol	67-63-0	0.16	0.02
106	Isopropyl Palmitate	142-91-6	0.034	0.034
7	Methane, dichlorofluoro-	75-43-4	0.0020	0.0030
1	Methyl nitrite	624-91-9	0.034	0.048
4	Methyl Alcohol	67-56-1	0.39	0.10
33	Methyl Isobutyl Ketone	108-10-1	0.0059	0.0053
15	Nitric acid, ethyl ester	625-58-1	0.037	0.004
20	Nitric acid, propyl ester	627-13-4	0.025	0.005
32	Nitric acid, ethyl ester	625-58-1	0.028	0.006

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
47	Nitric acid, butyl ester	928-45-0	0.030	0.014
59	Nitric acid, pentyl ester	1002-16-0	0.012	0.006
71	Nitric acid, hexyl ester	20633-11-8	0.0084	0.0073
74	Nitric acid, heptyl ester	20633-12-9	0.0032	0.0028
78	Nitric acid, hexyl ester	20633-11-8	0.0042	0.0036
85	Nitric acid, hexyl ester	20633-11-8	0.010	0.009
93	Nitric acid, decyl ester	2050-78-4	0.0058	0.0051
6	Nitrous acid, butyl ester	544-16-1	0.024	0.0003
12	Nitrous acid, butyl ester	544-16-1	0.012	0.001
19	Nitrous acid, butyl ester	544-16-1	0.028	0.005
90	Nonanenitrile	2243-27-8	0.0060	0.0052
68	Octanal	124-13-0	0.0042	0.0036
39	Octane, 2-chloro-	628-61-5	0.0016	0.0027
82	Octanenitrile	124-12-9	0.022	0.015
100	Pentadecane	629-62-9	0.0041	0.0036
48	Phenol	108-95-2	0.0021	0.0036
36	Propane, 2-methyl-2-nitro-	594-70-7	0.018	0.004
34	Propanoic acid	79-09-4	0.0046	0.0080
35	Pyrazine	290-37-9	0.0022	0.0038
62	Pyridine, 2,4-dimethyl-	108-47-4	0.0013	0.0022
44	Tetrachloroethylene	127-18-4	0.011	0.001
98	Tetradecane	629-59-4	0.020	0.018
9	Trichloromonofluoromethane	75-69-4	0.17	0.02
10	Trichloromonofluoromethane	75-69-4	0.013	0.023
Sum of Tentatively Identified Compounds:			2.6	

1 CAS = Chemical Abstract Service.

2 Average of 3, 4-L TST samples, values listed are estimates.

Table 4-9
Tank TX-118 Tentatively Identified Organic Compounds in TST Samples
Sorted by Estimated Concentration --
Analyses Conducted by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
4	Methyl Alcohol	67-56-1	0.39	0.10
16	1-Propanol	71-23-8	0.19	0.04
8	Ethanol	64-17-5	0.18	0.05
9	Trichloromonofluoromethane	75-69-4	0.17	0.02
11	Isopropyl Alcohol	67-63-0	0.16	0.02
53	3-Heptanone	106-35-4	0.14	0.04
72	1-Hexanol, 2-ethyl-	104-76-7	0.10	0.05
18	2-Butanone	78-93-3	0.087	0.035
77	1-Propanol, 2,2-dimethyl-, nitrate	926-42-1	0.048	0.008
2	1-Propene, 2-methyl-	115-11-7	0.043	0.007
63	3-Hepten-2-one, 4-methyl-	22319-25-1	0.040	0.016
54	3-Heptanol	589-82-2	0.037	0.012
15	Nitric acid, ethyl ester	625-58-1	0.037	0.004
105	Benzehesulfonamide, N-butyl-	3622-84-2	0.036	0.036
3	Butane	106-97-8	0.034	0.016
1	Methyl nitrite	624-91-9	0.034	0.048
106	Isopropyl Palmitate	142-91-6	0.034	0.034
47	Nitric acid, butyl ester	928-45-0	0.030	0.014
19	Nitrous acid, butyl ester	544-16-1	0.028	0.005
32	Nitric acid, ethyl ester	625-58-1	0.028	0.006
5	1-Propene, 2-methyl-	115-11-7	0.027	0.023
81	Acetophenone	98-86-2	0.026	0.019
20	Nitric acid, propyl ester	627-13-4	0.025	0.005
70	Cyclopentane, (2-methylpropyl)-	3788-32-7	0.024	0.012
76	Alkane		0.024	0.018
6	Nitrous acid, butyl ester	544-16-1	0.024	0.0003
21	Furan, tetrahydro-	109-99-9	0.024	0.003

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
65	1-Heptanol	111-70-6	0.023	0.007
82	Octanenitrile	124-12-9	0.022	0.015
38	1-Pentanol	71-41-0	0.022	0.005
79	1-Octanol	111-87-5	0.021	0.010
103	Diethyl Phthalate	84-66-2	0.020	0.007
98	Tetradecane	629-59-4	0.020	0.018
40	2-Pentanone, 4,4-dimethyl-	590-50-1	0.020	0.002
75	1H-Pyrozole, 4,5-dihydro-1, 5-dimethyl- and others		0.010	0.018
36	Propane, 2-methyl-2-nitro-	594-70-7	0.018	0.004
64	Alkenol		0.018	0.005
61	4-Hydroxy-4-methylpentanone		0.018	0.006
83	2-Nonanone	821-55-6	0.017	0.021
30	2-Butanone, 3,3-dimethyl-	75-97-8	0.015	0.002
52	Alkenol		0.014	0.002
50	1-Hexanol	111-27-3	0.014	0.0036
17	3-Buten-2-one	78-94-4	0.013	0.002
10	Trichloromonofluoromethane	75-69-4	0.013	0.023
101	Hexadecanoic acid	57-10-3	0.012	0.020
12	Nitrous acid, butyl ester	544-16-1	0.012	0.001
59	Nitric acid, pentyl ester	1002-16-0	0.012	0.006
44	Tetrachloroethylene	127-18-4	0.011	0.001
80	Heptane, 2,2,4,6,6-pentamethyl-	13475-82-6	0.011	0.008
27	3-Pentanone	96-22-0	0.011	0.010
51	4-Heptanone	123-19-3	0.011	0.0031
84	Benzene, nitro-	98-95-3	0.010	0.009
85	Nitric acid, hexyl ester	20633-11-8	0.010	0.009
71	Nitric acid, hexyl ester	20633-11-8	0.0084	0.0073
60	2,2'-Bioxepane	74793-02-5	0.0080	0.0071

WHC-SD-WM-ER-449 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
91	C10-Alkanone		0.0073	0.0064
89	1-Nonanol	143-08-8	0.0071	0.0061
26	2-Butenenitrile	4786-20-3	0.0071	0.0004
45	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0071	0.0062
97	Decane, 5-ethyl-5-methyl-	17312-74-2	0.0066	0.0057
24	2-Butenal, (E)-	123-73-9	0.0064	0.0057
90	Nonanenitrile	2243-27-8	0.0060	0.0052
33	Methyl Isobutyl Ketone	108-10-1	0.0059	0.0053
93	Nitric acid, decyl ester	2050-78-4	0.0058	0.0051
14	2-Propanol, 2-methyl-	75-65-0	0.0054	0.0094
41	3-Hexanone	589-38-8	0.0051	0.0013
104	1,1'-Biphenyl, 3,3'-dichloro-	2050-67-1	0.0050	0.0044
73	C3-Cyclohexane		0.0050	0.0044
58	3-Heptanone, 6-methyl-	624-42-0	0.0050	0.0010
42	1-Hexanol	111-27-3	0.0049	0.0084
96	Decanenitrile	1975-78-6	0.0047	0.0040
94	Decane, 2-methyl-	6975-98-0	0.0047	0.0041
28	2-Heptene, (E)-	14686-13-6	0.0047	0.0041
102	1,1'-Biphenyl, 3-chloro-	2051-61-8	0.0047	0.0041
34	Propanoic acid	79-09-4	0.0046	0.0080
23	3-Butenenitrile	109-75-1	0.0046	0.0040
68	Octanal	124-13-0	0.0042	0.0036
78	Nitric acid, hexyl ester	20633-11-8	0.0042	0.0036
100	Pentadecane	629-62-9	0.0041	0.0036
67	2,2,4-Trimethyl-3-pentanone	5857-36-3	0.0040	0.0004
55	Heptanal	111-71-7	0.0039	0.0033
88	Dodecane, 4-methyl-	6117-97-1	0.0039	0.0034
46	Acetic acid, butyl ester	123-86-4	0.0033	0.0057

WHC-SD-WM-ER-449 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
86	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.0033	0.0028
74	Nitric acid, heptyl ester	20633-12-9	0.0032	0.0028
87	Heptane, 3-ethyl-5-methyl-	52896-90-9	0.0032	0.0028
49	Cyclohexane, 1,1-dimethyl-	590-66-9	0.0031	0.0027
99	Biphenyl	92-52-4	0.0029	0.0025
31	2-Heptene, (E)-	14686-13-6	0.0025	0.0043
25	2-Butanone, 3-methyl-	563-80-4	0.0024	0.0042
37	3-Pentanone, 2-methyl-	565-69-5	0.0024	0.0041
29	1H-Pyrazole, 1-methyl-	930-36-9	0.0022	0.0038
35	Pyrazine	290-37-9	0.0022	0.0038
48	Phenol	108-95-2	0.0021	0.0036
22	Butane, 1-chloro-	109-69-3	0.0021	0.0037
69	Benzonitrile	100-47-0	0.0020	0.0034
7	Methane, dichlorofluoro-	75-43-4	0.0020	0.0030
13	2-Propenenitrile	107-13-1	0.0020	0.0040
95	1-Undecanol	112-42-5	0.0018	0.0031
39	Octane, 2-chloro-	628-61-5	0.0016	0.0027
57	Cyclobutanone, 3,3-dimethyl-	1192-33-2	0.0016	0.0027
56	Cyclopent-2-ene-1-one, 2,3,4-trimethyl-	83321-16-8	0.0015	0.0026
92	2-Oxazolidinone, 5-methyl-3-(2-propenyl)-	55956-20-2	0.0014	0.0024
66	Cyclohexane, 1-ethyl-4-methyl-, trans-	6236-88-0	0.0014	0.0024
62	Pyridine, 2,4-dimethyl-	108-47-4	0.0013	0.0022
43	2-Furanmethanol, tetrahydro-5-methyl-, trans-	54774-28-6	0.0011	0.0019
Sum of Tentatively Identified Compounds:			2.6	

¹ CAS = Chemical Abstract Service.

² Average of 3, 4-L TST samples, values listed are estimates.

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