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Title/Desc:

TANK 241C108 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
7/1993 & 8/1994

ENGINEERING CHANGE NOTICE

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Page 2 of 2

1. ECN (use no. from pg. 1)

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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	☐
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Radiation Work Permit	☐	Essential Material Specification	☐	Purchase Requisition	☐
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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-C-108 Headspace Gas and Vapor Characterization Results for Samples Collected in July 1993 and August 1994

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Acronyms and Abbreviations

CES	consensus exposure standard
EPA	Environmental Protection Agency
GC	gas chromatograph
GC/MS	gas chromatograph/mass spectrometer
ISS	<i>in situ</i> sampling
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-C-108 Headspace Gas and Vapor Characterization Results
for Samples Collected in July 1993 and August 1994

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank C-108 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 August 1994 sampling event, but also includes selected results of the July 1993 sampling event. The tank C-108 headspace was sampled in July 1993 to address concerns about hydrogen cyanide fugitive emissions from the waste tanks (Saget 1992), and in August 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 were 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 C-108, 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 C-108 was vapor sampled in July 1993 and July 1994 using *in situ* sampling (ISS) methods. In the July 1993 sampling event, liquid-filled bubblers were lowered into the tank headspace to sample for hydrogen cyanide. The second ISS event, in July 1994, was performed as required by *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991). In the July 1994 event, sorbent traps lowered into the tank headspace were contaminated with radioactive particles, and could not be analyzed.

Tank C-108 was sampled again in August 1994 using the more robust Vapor Sampling System (VSS). Because there are discrepancies between results from the ISS and VSS methods that are not understood (Huckaby 1994a), results from early ISS events are generally considered to be less valid than results from the VSS events. Nevertheless, a brief description of the July 1993 ISS event and the results of the hydrogen cyanide sampling 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. All other results presented here are from the August 1994 VSS sampling event.

Samples collected are thought to have been representative of the tank C-108 headspace when the tank was sampled, and sample analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents (Meacham et al. 1995). No assessment has been made of how the tank C-108 headspace composition changes with time, though studies of tank C-103 suggest that composition changes probably occur very slowly in the passively ventilated tanks (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank C-108 is the second tank in a 3-tank cascade with tanks C-107 and C-109, and is connected to both tanks C-107 and C-109 via 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long cascade lines. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank C-107 or tank C-109 may be transferred to tank C-108 (unless the cascade lines are obstructed). However, headspace data, as discussed in Section 3.5, indicate that the inter-tank exchange of gases and vapors has little effect on the headspace composition of tank C-108.

The cascade of tanks C-107, C-108, and C-109 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 July 1993 *In Situ* Sampling Event

Tank C-108 was sampled using ISS methods on July 23, 1993 by WHC Sampling and Mobile Laboratories. This sampling was conducted to address concerns that ferrocyanide Watch List tanks could be releasing hydrogen cyanide vapors into the breathing zone of tank farm workers (Saget 1992). Samples for hydrogen cyanide were collected from a point approximately 7.8 m below the top of the flange on riser 3, between 2:00 p.m. and 3:30 p.m.

Huckaby et al. (1995) give a general description of the ISS method and equipment. Pingel (1993) provides field sampling information for the tank C-108 June 1993 ISS event. In addition to the hydrogen cyanide results presented below, Lerner and Pool (1994) provide sample preparation and analysis results for selected organic and inorganic vapors.

2.2 August 1994 Vapor Sampling System Sampling Event

Headspace gas and vapor samples were collected from tank C-108 using the VSS on August 5, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by the sample and analysis plan¹ (WHC 1995b, Appendix A). The tank headspace temperature was determined to be 25 °C. Air from the tank C-108 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 4, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), Pacific Northwest Laboratories (PNL), and Oregon Graduate Institute of Science and Technology (OGIST) through a contract with Sandia National Laboratories. The 39 tank air samples and 2 ambient air control samples collected are listed in Table 2-1 by analytical laboratory. Table 2-1 also lists the 18 trip blanks 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).

¹ The current requirement that sampling and analysis parameters be specified by a tank characterization plan was not in effect for gas and vapor sampling until October 1, 1994.

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,2} 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 and are given in Section 3.3. Inorganic analyte sorbent traps were prepared and analyzed by PNL. All PNL results were produced at PNL quality assurance impact level 3. SUMMATM canister samples were prepared and analyzed by OGIST. OGIST was not operating under a WHC-approved quality assurance plan when samples were analyzed, so OGIST data have been placed in square brackets both in Table 3-1 and elsewhere in the report to indicate that they represent secondary results. Reports by Lucke et al. (1995) and Rasmussen (1994) describe sample preparation and analyses.

OGIST SUMMATM canister analyses were began 14 days after the samples were collected, PNL analyses of the ISS hydrogen cyanide samples was performed 6 days after these samples were collected, and all PNL inorganic vapor sorbent traps from the VSS sampling event were performed within 14 days after sample collection (Rasmussen 1994, Ligotke 1995). The 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994) was consequently satisfied. The 60-day holding time was administratively chosen, and no holding time study has been done to address the stability of analytes in SUMMATM canisters in the chemical matrix of tank samples.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Ammonia concentration in the headspace of tank C-108 was determined to be 2.7 ppmv. This is the lowest ammonia concentration measured in any passively ventilated tank. The relatively low ammonia concentration in tank C-108 may be related to the fact that only a small quantity of relatively cool waste is stored in tank C-108. Given the LFL of ammonia in air is about 15 by volume (vol%), the measured 2.7 ppmv corresponds to about 0.002 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The tank C-108 hydrogen concentration was measured to be an average [15.3 ppmv] in 3 OGIST SUMMATM samples. In general, hydrogen is of concern as a fuel. The measured [15.3 ppmv] of hydrogen in tank C-108, however, represents only about 0.04 % of the LFL for hydrogen in air, and is not a flammability concern at this level.

Nitrous oxide was measured to be present in the 3 OGIST SUMMATM samples at an average [344 ppmv]. This is higher than has typically been measured in other passively ventilated tanks that have been sampled, but higher values have also been measured. 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 C-108 headspace.

3.2 Carbon Dioxide and Carbon Monoxide

² SUMMA is a trademark of Moleetrics, Inc., Cleveland, Ohio.

The average measured headspace carbon dioxide concentration, [16.3 ppmv], is markedly lower than normal ambient air concentrations. In ambient air carbon dioxide is typically present at 350 to 400 ppmv, and typically lower than this 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 monoxide in the tank C-108 headspace, at about [0.10 ppmv], is about the same as in ambient air, where it typically ranges from 0.05 to 0.15 ppmv. Elevated waste tank headspace carbon monoxide concentrations are common (e.g., carbon monoxide concentration³ in tank C-103 was [26.7 ppmv], Huckaby and Story 1994), and are thought to be due to the decomposition of organic waste in the tanks. The relatively low carbon monoxide in tank C-108 may be due to the fact that the tank has a relatively small, cool waste inventory.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank C-108 headspace were determined to be 0.24 ppmv and ≤ 0.04 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank C-108. 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 C-108 headspace.

The water vapor concentration of tank C-108 was determined to be about 17.5 mg/L, at the tank headspace temperature of 25 °C and pressure of 990 mbar (743 torr), (WHC 1995b). This corresponds to water vapor partial pressure of 24.1 mbar (18.1 torr), to a dew point of 20.5 °C, and to a relative humidity of 76 %.

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 liquid-filled bubblers for hydrogen cyanide indicated the concentration of this analyte to be below 0.0003 ppmv in all 3 samples. 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 C-108. 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

³ The carbon monoxide measurement in tank C-103 was made by OGIST, and should be considered secondary data.

Aside from water vapor, the most abundant waste constituent in the tank C-108 headspace is nitrous oxide. Nitrous oxide, ammonia, and hydrogen have been detected in most tank headspaces sampled to date and are usually the dominate waste species. The concentration of nitrous oxide in tank C-108 is above the average for other tanks that have been sampled, but the hydrogen concentration in tank C-108 is relatively low, and the ammonia concentration is very low.

The small relative standard deviations of the results, given in the last column in Table 3-1, indicate the precision of reported results is good. Relative standard deviations range from 0.3 % for nitrous oxide results, to 30 % for carbon monoxide results. The larger relative standard deviation of the carbon monoxide results is due to the fact that it is near the analytical method's limit of quantitation. 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.), and the small relative standard deviations suggest a high degree of control was maintained both in the field and in the laboratories.

As discussed briefly in Section 1.3, it is possible that gases and vapors generated by the waste in tanks C-107 and C-109 could be transferred to tank C-108 via the cascade lines. Table 3-2 lists the measured concentrations of selected inorganic gases and vapors in tanks C-107, C-108, and C-109. If a significant exchange of gases and vapors were taking place between adjacent tanks, either their headspace compositions would be very similar, or all constituents detected in one tank would be at equal or higher concentration in the other tank. Consideration of the data in Table 3-2 indicates that any transfer of gases and vapors between these tanks is probably negligible. Specifically, hydrogen is at much higher concentrations in tanks C-107 and C-109 than in tank C-108, and nitrous oxide is at a much higher concentration in tank C-108 than in tank C-107.

4.0 ORGANIC VAPORS

Organic vapors in the tank C-108 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. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1994) and Lucke et al. (1995). Quantitative measurements of the methane concentration and the total nonmethane organic carbon (TNMOC) concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method were also performed by OGIST (EPA 1988, Rasmussen 1994).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank C-108. PNL results were produced at PNL quality assurance impact level 3. PNL SUMMA™ analyses were not completed until 62 days after sample collection. This exceeded the administratively chosen 60-day holding time (Keller 1994). 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. Similarly, the OGIST methane and TNMOC measurements were conducted in the absence of a WHC-approved quality assurance project plan, and should be considered secondary data.

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 Analytes

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 by analysis of standards. 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 included 40 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988), plus 14 analytes selected mainly from the toxicology panel's review of vapor data on tank C-103.

Given in Table 4-1 are the organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL and OGIST. PNL performed analyses according to the EPA TO-14 methodology (EPA 1988, Lucke et al. 1995). Only 2 of the 40 TO-14 analytes were observed to be above the 0.002 ppmv quantitation limit of the analyses, and 1 of these analytes, 1,1,2-trichloro-1,2,2-trifluoroethane, is thought to be a contaminant of analysis (Lucke et al. 1995). The results for methane are those of OGIST (Rasmussen 1994). Averages reported are from analyses of 3 SUMMA™ canister samples except where noted.

Jenkins et al. (1995a) report the positive identification of 17 of 27 analytes in TST samples. Despite calibration of the instrument over a 20-fold concentration range, only 1 analyte was quantitated in all 5 of the TST samples. All positively identified analytes, and their average concentrations from the analysis of 5 TSTs, are given in Tables 4-2, 4-3, and 4-4. Table 4-2 lists the single positively identified, quantitated analyte, Table 4-3 lists the positively identified analytes which were not quantitated (because the measurement was outside the calibration range for at least 1 sample), and Table 4-4 lists the single positively identified analyte which exceeded its practical holding time. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so that no analyte appears in more than 1 of these tables. Data in Tables 4-3 and 4-4 should not be considered quantitative and 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, 1-butanol exceeded its practical holding time, and may have been affected by the 25 day period between sample collection and analysis. Jenkins et al. (1995b) describe the ORNL practical holding time study, and report the practical holding time of 1-butanol is 17 days. It should be noted that the contractual holding time for the TST samples was 60 days.

Three target analytes were common to both the ORNL and PNL analyses: Dichloromethane, benzene, and toluene. The PNL and ORNL results for these analytes are given Table 4-5 for comparison. Neither ORNL nor PNL detected dichloromethane. ORNL detected trace amounts of benzene and toluene, but these were both below the 0.002 ppmv limit of detection of PNL.

The 2 most abundant analytes in Tables 4-1 through 4-4 are methane and propanone. At 0.32 ppmv, the methane concentration in tank C-111 is at about the level it is in ambient air, and does not present a flammability risk. Similarly, propanone, at 0.018 ppmv, presents no flammability risks.

4.2 Tentatively Identified Organic Analytes

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 standards of 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 (e.g., molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (e.g., butanal) from SUMMA™ samples has been problematic.

The PNL list of tentatively identified compounds, with estimated concentrations, is given in Table 4-6, and the ORNL list of tentatively identified compounds, and their estimated concentrations, is given in Table 4-7. Because the list of tentatively identified organic compounds in TST samples is long and finding any given compound may be difficult, the list has been sorted alphanumerically by compound name in Table 4-8. Table 4-9 gives the same list, sorted in order of decreasing estimated concentration. Numbers in the first columns of Tables 4-8 and 4-9 (Cmpd #) identify the location of the compound in Table 4-7. Estimated concentrations given in Tables 4-6 through 4-9 are in mg/m³, based on dry air at 0 °C and 1.01 bar.

The PNL and ORNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Lucke et al. (1995), respectively, and should be reviewed before this data are used for decision making. 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 # 30 and 32 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.

Concentrations given in Tables 4-6 and 4-7 should be considered rough estimates. 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.

4.3 Total Nonmethane Organic Carbon

OGIST measured the TNMOC concentration in 3 SUMMA™ canister samples using the EPA TO-12 method (Rasmussen 1994). The sample mean was [0.35 mg/m³], with a standard deviation of [0.02 mg/m³]. The TNMOC is very low in tank C-108 compared to other tanks that have been sampled. For comparison, the TNMOC concentration in clean ambient air may range from 0.030 to 0.100 mg/m³.

4.4 Discussion of Organic Analytes

Some of the compounds listed in Tables 4-1 through 4-7 were introduced to the tank with process waste streams, and are detected in the headspace because the original inventory has not been completely evaporated or degraded. Examples of these are tributyl phosphate, which was used as an extractant in several Hanford processes; dibutyl butylphosphonate, which was a contaminant of tributyl phosphate; and the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-undecane, n-dodecane, n-tridecane, and n-pentadecane) that were used as diluents of tributyl phosphate. Notably absent from the tank C-108 headspace are the semivolatile cyclic alkanes (e.g., methylated decahydronaphthalenes, cyclopentanes, and cyclohexanes) that have been associated with the NPHs in the 241-BY tank farm and several of the tanks in 241-C farm.

Most of the compounds in Tables 4-1 through 4-9 are believed to be chemical reaction and radiolytic reaction products of the semivolatile or nonvolatile organic waste stored in the tank. For example, 1-

butanol is known to be formed by the hydrolysis of tributyl phosphate, and it has been suggested that the alcohols, aldehydes, ketones, nitriles, alkenes, and short chain alkanes are all degradation products of NPHs.

Examination of the compounds listed in Tables 4-1 through 4-9 suggests many of the volatile species (presumed to be degradation products of the NPHs) have functional groups on the molecule's first or second carbon atom. For example, most alkenes listed have their double bond between the first and second carbon atoms, and ketones generally have the double bonded oxygen atom on the second carbon atom.

Though their concentrations are not significant, many alcohols and acids were tentatively identified by ORNL (Tables 4-7 and 4-8). These have generally not been observed to be as numerous in other NPH-rich tank headspaces, which tend to be dominated by aldehydes, ketones, and alkenes.

5.0 SUMMARY

The tank C-108 headspace was sampled in July 1993 and August 1994 for gases and vapors to address flammability and industrial hygiene concerns. Results unique to the July 1993 event and essentially all results from the August 1994 event have 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 1995).

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Table 2-1
Tank C-108 Gas and Vapor Sample Type and Number for August 1994 Sampling Event

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	2.0	Organic vapors	4 tank air samples
		4.0	Organic vapors	4 tank air samples + 6 trip blanks
Oregon Graduate Institute of Science and Technology	SUMMA™ canister	6.0	Hydrogen, Nitrous Oxide, Carbon Dioxide, Carbon Monoxide	3 tank air samples
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blanks
	Oxidation bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	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
Analyses by Oregon Graduate Institute of Science and Technology and by Pacific Northwest Laboratory
Tank C-108 Inorganic Gas and Vapor Concentrations --

Compound	CAS ¹ Number	Sample Type	Number of samples	Average ² (ppmv)	Standard Deviation ² (ppmv)	RSD ^{2,3} (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	2.7	0.3	11
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	[16.3]	[1.5]	[9]
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	[0.10]	[0.03]	[30]
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	[15.3]	[1.2]	[8]
Hydrogen Cyanide ⁴ , HCN	74-90-8	Sorbent Trap	3	< 0.0003	—	—
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.24	0.01	4
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.04	—	—
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	[344]	[1]	[0.3]
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	24,300 (17.5 mg/L)	2,100 (1.5 mg/L)	10

¹ CAS = Chemical Abstracts Service.

² Bracketed values are from OGIST and should be considered secondary results, non-bracketed values are from PNL and should be considered primary results.

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

⁴ Results for hydrogen cyanide are from the July 1993 ISS event (Lerner and Pool 1994).

Table 3-2
Comparison of Tank C-107, C-108, and C-109 Headspace Constituents --
Inorganic Analyses by Oregon Graduate Institute of Science and Technology,
and Organic Analyses by Oak Ridge National Laboratory¹

Tank:	C-107 ²	C-108	C-109 ³
Date sampled, (mo/day/yr)	9/9/94	8/5/94	8/10/94
Headspace temperature, (°C)	45.9	25	27
Ammonia, (ppmv)	84	2.7	10.1
Hydrogen, (ppmv)	[230]	[15.3]	[125]
Carbon dioxide, (ppmv)	[725]	[16.3]	[3]
Carbon monoxide, (ppmv)	[1.7]	[0.10]	[0.41]
Nitric oxide, (ppmv)	0.20	0.24	0.51
Nitrogen dioxide, (ppmv)	≤ 0.02	≤ 0.04	≤ 0.06
Nitrous oxide, (ppmv)	[78]	[344]	[369]
Water vapor, (mg/m ³)	70.7	17.5	20.4
Water vapor, (% relative humidity)	86	76	79
Ethanenitrile (acetonitrile), (ppmv)	(0.25)	(0.0052)	(0.26)
Propanone (acetone), (ppmv)	(0.094)	0.018	(0.012)
1-Butanol, (ppmv)	(0.0025)	(0.00049)	0.0032
n-Dodecane, (ppmv)	0.0073	(0.00053)	(0.00026)
n-Tridecane, (ppmv)	0.0092	(0.0011)	(0.00047)
Total nonmethane organic compounds by EPA TO-12 method, (mg/m ³)	[3.6]	[0.35]	[0.65]

¹ Where PNL inorganic gas or vapor data was unavailable for tanks C-108 and C-109, OGIST results are given in brackets to indicate the data should be considered secondary results. Organic vapor results are from ORNL, with semiquantitative values in parentheses and quantitative values not in parentheses.

² Data are from Huckaby 1995a.

³ Data are from Huckaby 1994b.

Table 4-1
Tank C-108 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	[0.67]	[0.01]	[0.1]
2	Trichlorofluoromethane	75-69-4	0.0095	0.00014	2
3	1,1,2-Trichloro-1,2,2-trifluoroethane ⁵	76-13-1	0.0087	0.00060	7
4	Benzene	71-43-2	<0.002	--	--
5	Toluene	108-88-3	<0.002	--	--

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 by OGIST and should be considered a secondary result (Ramussen 1994a).

5 Suspect contamination.

Table 4-2
Tank C-108 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	Propanone (acetone)	67-64-1	0.018	0.019	110

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

2 CAS = Chemical Abstract Service.

3 Average of 5 TST samples: 3 were 4-L and 2 were 1-L.

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

Table 4-3
Tank C-108 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	0.0052	0.0032	61
2	n-Hexane	110-54-3	0.00029	0.00064	224
3	Benzene	71-43-2	0.00038	0.00030	79
4	n-Heptane	142-82-5	0.00013	0.00030	224
5	Toluene	108-88-3	0.00024	0.00047	192
6	2-Hexanone	591-78-6	0.00012	0.00024	193
7	n-Octane	111-65-9	0.00014	0.00028	201
8	2-Heptanone	110-43-0	0.00016	0.00028	174
9	n-Nonane	111-84-2	0.00021	0.00028	136
10	n-Octanenitrile	124-12-9	0.000012	0.000026	224
11	n-Nonanenitrile	2243-27-8	0.000081	0.000077	95
12	n-Dodecane	112-40-3	0.00053	0.00058	110
13	n-Tridecane	629-50-5	0.0011	0.0011	97
14	Dibutyl butylphosphonate	75-46-4	0.000008	0.000004	55
15	Tributyl phosphate	126-73-8	0.000075	0.000069	92

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 5 TST samples: 3 were 4-L and 2 were 1-L.

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

Table 4-4
Tank C-108 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	1-Butanol ⁵	71-36-3	0.00049	0.00060	121

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

2 CAS = Chemical Abstract Service.

3 Average of 5 TST samples: 3 were 4-L and 2 were 1-L.

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.

Table 4-5
Tank C-108 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 ¹ Average ³ (ppmv)	PRD ⁴ (%)
Benzene	71-43-2	0.00038	< 0.002	--
Toluene	108-88-3	0.00024	< 0.002	--

1 CAS = Chemical Abstract Service.

2 Average of 5 TST samples: 3 were 4-L and 2 were 1-L.

3 Average of 3 samples.

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

Table 4-6
Tank C-108 Tentatively Identified Organic Compounds in SUMMA™ Samples --

Cmpd #	Compound	CAS ¹ Number	Average ² mg/m ³	Standard Deviation mg/m ³
1	Ethanenitrile (acetaldehyde)	75-07-0	0.10	0.02
2	Propanone (acetone)	67-64-1	0.09	0.03
Sum of tentatively identified compounds:			0.19	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples; presented values are estimates.

Table 4-7
Tank C-108 Tentatively Identified Organic Compounds in TST Samples
in Order of Chromatographic Elution --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	1-Butene	106-98-9	0.038	0.053
2	Methane, trichlorofluoro	75-69-4	0.042	0.032
3	Acetic Acid	64-19-7	0.083	0.117
4	Acetic Acid	64-19-7	0.038	0.085
5	Propanoic acid	79-09-4	0.003	0.008
6	Hexanal	66-25-1	0.010	0.023
7	Cyclotrisiloxane, hexamethyl	541-05-9	0.026	0.020
8	Alkanone		0.012	0.026
9	Heptanal	111-71-7	0.009	0.021
10	4H-1,2,4-Triazol-3-amine, 4-ethyl	42786-06-1	0.004	0.006
11	Ethanol, 2-Butoxy	111-76-2	0.001	0.001
12	Cyclobutane, 1,1,2,3,3-pentamethyl	57905-86-9	0.002	0.004
13	Cyclotetrasiloxane, octamethyl	556-67-2	0.020	0.026
14	Benzene, (1-methylethenyl)-	98-83-9	0.001	0.002
15	Octanal	124-13-0	0.016	0.029
16	1-Hexanol, 2-Ethyl	104-76-7	0.006	0.005
17	1-Octanol	111-87-5	0.004	0.009
18	Ethanone, 1-phenyl	98-86-2	0.001	0.001
19	Benzenemethanol, a,a-dimethyl	617-94-7	0.006	0.002
20	Nonanal	124-19-6	0.018	0.024
21	Benzoic acid, 2-[trimethylsilyl]oxy]-trimeth	3789-85-3	0.002	0.002
22	1-Nonanol	143-08-8	0.002	0.003
23	Decanal	112-31-2	0.011	0.013
24	Benzenamine, N-phenyl	122-39-4	0.001	0.002
25	1,3,5,7-Tetraazatricyclo[3.3.1.1 ^{3,7}]decane	100-97-0	0.001	0.002

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
26	2,5-Pyrrolidinedione, 1-methyl	1121-07-9	0.001	0.001
27	Undecanal	112-44-7	<0.001	--
28	Decanoic acid	334-48-5	<0.001	--
29	Alkane		<0.001	--
30	Butanoic acid, butyl ester and siloxane	109-21-7	<0.001	--
31	Alkane		0.002	0.002
32	Butanoic acid, butyl ester	109-21-7	<0.001	--
33	n-Tetradecane	629-59-4	0.002	0.003
34	Dodecanal	112-54-9	<0.001	--
35	Mixture		<0.001	--
36	Decane, 1,1'-oxybis	2456-28-2	<0.001	--
37	5,9-Undecadio-2-one, 6,10-dimethyl-, (Z)	3879-26-3	0.002	0.002
38	2,5-Cyclohexadiene, 1,4-dione, 2,6-bis(1	719-22-2	<0.001	--
39	Alkanol and alkyl benzene		0.001	0.002
40	C12-Alkene		0.003	0.002
41	Alkene		<0.001	--
42	2,5-Cyclohexadiene-1,4-dione, 2,6-bis	719-22-2	0.002	0.002
43	n-Hexadecane	544-76-3	0.001	0.001
44	Tetradecanoic acid	544-63-8	0.002	0.004
45	Decanoic acid	334-48-5	<0.001	--
46	Dodecanoic acid	143-07-7	0.010	0.007
47	n-Tetradecane	629-59-4	<0.001	--
48	Dodecane, 2-methyl-6-propyl	55045-08-4	0.003	0.004
49	Propanoic acid, 2-methyl-1(1,1-dimethyle	74381-40-1	0.017	0.009
50	Benzenamine, N-phenyl	122-39-4	0.009	0.006
51	Hexadecanamide	629-54-9	0.001	0.001
52	N-Hexyl-benzene-sulfonamide		0.003	0.003
53	para-T-Butyl Benzoic acid, methyl ester		0.002	0.003

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
54	1,2-Benzenedicarboxylic acid, bis-(2ethyl	117-81-7	0.001	0.002
55	Octadecanoic acid	57-11-4	0.001	0.002
56	Mixture		0.001	0.002
57	1-Hexadecanol and others		0.002	0.003
58	Mixture (alkane and alkanoic acid)		0.002	0.002
59	Mixture		0.002	0.002
60	9-Octadecenoic acid, (Z)-	112-80-1	0.003	0.004
61	1,1'-Biphenyl, 2,2'-diethyl	13049-35-9	0.001	0.001
62	Tetradecanoic acid	544-63-8	0.055	0.037
63	Benzenesulfonamide, N-butyl	3622-84-2	0.132	0.103
64	Tetradecanoic acid, 12-methyl, (S)	5746-58-7	0.005	0.004
65	Cyclohexanol, 1,1'-dioxybis-and others		<0.001	--
66	Pentadecanoic acid	1002-84-2	0.023	0.016
67	C14-Alkene		0.016	0.028
68	1-Hexadecanol	36653-82-4	0.012	0.020
69	Alkanol		0.001	0.003
70	n-Hexadecane	544-76-3	0.001	0.002
71	Alkane		0.004	0.010
72	9-Hexadecenoic acid	2091-29-4	0.062	0.052
73	Hexadecanoic acid	57-10-3	0.120	0.088
74	1,2-Benzenedicarboxylic acid, butyl 2-me	17851-53-5	0.004	0.006
75	Alkanol		<0.001	--
76	1-Hexadecanol	36653-82-4	0.001	0.003
77	1-Hexadecanol, acetate	629-70-9	0.002	0.004
78	1-Hexadecanol, 2-methyl	2490-48-4	0.002	0.002
79	Hexadecanoic acid	57-10-3	0.002	0.004
80	Hexadeanoic acid, 1-methylethyl ester	142-91-6	0.007	0.006
Sum of tentatively identified compounds:			0.881	

1 CAS = Chemical Abstract Service.

2 Average of 5 TST samples; 3 were 4-L and 2 were 1-L; presented values are estimates.

Table 4-8
Tank C-108 Tentatively Identified Organic Compounds in TST Samples
Sorted Alphanumerically --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	1-Butene	106-98-9	0.038	0.053
78	1-Hexadecanol, 2-methyl	2490-48-4	0.002	0.002
76	1-Hexadecanol	36653-82-4	0.001	0.003
57	1-Hexadecanol and others		0.002	0.003
22	1-Nonanol	143-08-8	0.002	0.003
68	1-Hexadecanol	36653-82-4	0.012	0.020
17	1-Octanol	111-87-5	0.004	0.009
16	1-Hexanol, 2-Ethyl	104-76-7	0.006	0.005
77	1-Hexadecanol, acetate	629-70-9	0.002	0.004
61	1,1'-Biphenyl, 2,2'-diethyl	13049-35-9	0.001	0.001
54	1,2-Benzenedicarboxylic acid, bis-(2ethyl	117-81-7	0.001	0.002
74	1,2-Benzenedicarboxylic acid, butyl 2-me	17851-53-5	0.004	0.006
25	1,3,5,7-Tetraazatricyclo[3.3.1.1 ^{3,7}]decane	100-97-0	0.001	0.002
26	2,5-Pyrrolidinedione, 1-methyl	1121-07-9	0.001	0.001
38	2,5-Cyclohexadiene, 1,4-dione, 2,6-bis(1	719-22-2	<0.001	--
42	2,5-Cyclohexadiene-1,4-dione, 2,6-bis	719-22-2	0.002	0.002
10	4H-1,2,4-Triazol-3-amine, 4-ethyl	42786-06-1	0.004	0.006
37	5,9-Undecadio-2-one, 6,10-dimethyl-, (Z)	3879-26-3	0.002	0.002
60	9-Octadecenoic acid, (Z)-	112-80-1	0.003	0.004
72	9-Hexadecenoic acid	2091-29-4	0.062	0.052
3	Acetic Acid	64-19-7	0.083	0.117
4	Acetic Acid	64-19-7	0.038	0.085
29	Alkane		<0.001	--
31	Alkane		0.002	0.002
71	Alkane		0.004	0.010
39	Alkanol and alkyl benzene		0.001	0.002

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
69	Alkanol		0.001	0.003
75	Alkanol		<0.001	--
8	Alkanone		0.012	0.026
41	Alkene		<0.001	--
24	Benzenamine, N-phenyl	122-39-4	0.001	0.002
50	Benzenamine, N-phenyl	122-39-4	0.009	0.006
14	Benzene, (1-methylethenyl)-	98-83-9	0.001	0.002
19	Benzenemethanol, a,a-dimethyl	617-94-7	0.006	0.002
63	Benzenesulfonamide, N-butyl	3622-84-2	0.132	0.103
21	Benzoic acid, 2-[trimethylsilyl]oxy]-trimeth	3789-85-3	0.002	0.002
30	Butanoic acid, butyl ester and siloxane	109-21-7	<0.001	--
32	Butanoic acid, butyl ester	109-21-7	<0.001	--
40	C12-Alkene		0.003	0.002
67	C14-Alkene		0.016	0.028
12	Cyclobutane, 1,1,2,3,3-pentamethyl	57905-86-9	0.002	0.004
65	Cyclohexanol, 1,1'-dioxybis-and others		<0.001	--
13	Cyclotetrasiloxane, octamethyl	556-67-2	0.020	0.026
7	Cyclotrisiloxane, hexamethyl	541-05-9	0.026	0.020
23	Decanal	112-31-2	0.011	0.013
36	Decane, 1,1'-oxybis	2456-28-2	<0.001	--
28	Decanoic acid	334-48-5	<0.001	--
45	Decanoic acid	334-48-5	<0.001	--
34	Dodecanal	112-54-9	<0.001	--
48	Dodecane, 2-methyl-6-propyl	55045-08-4	0.003	0.004
46	Dodecanoic acid	143-07-7	0.010	0.007
11	Ethanol, 2-Butoxy	111-76-2	0.001	0.001
18	Ethanone, 1-phenyl	98-86-2	0.001	0.001
9	Heptanal	111-71-7	0.009	0.021

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
80	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.007	0.006
51	Hexadecanamide	629-54-9	0.001	0.001
73	Hexadecanoic acid	57-10-3	0.120	0.088
79	Hexadecanoic acid	57-10-3	0.002	0.004
6	Hexanal	66-25-1	0.010	0.023
2	Methane, trichlorofluoro	75-69-4	0.042	0.032
35	Mixture		<0.001	--
56	Mixture		0.001	0.002
58	Mixture (alkane and alkanoic acid)		0.002	0.002
59	Mixture		0.002	0.002
52	N-Hexyl-benzene-sulfonamide		0.003	0.003
43	n-Hexadecane	544-76-3	0.001	0.001
70	n-Hexadecane	544-76-3	0.001	0.002
33	n-Tetradecane	629-59-4	0.002	0.003
47	n-Tetradecane	629-59-4	<0.001	--
20	Nonanal	124-19-6	0.018	0.024
55	Octadecanoic acid	57-11-4	0.001	0.002
15	Octanal	124-13-0	0.016	0.029
53	para-T-Butyl Benzoic acid, methyl ester		0.002	0.003
66	Pentadecanoic acid	1002-84-2	0.023	0.016
5	Propanoic acid	79-09-4	0.003	0.008
49	Propanoic acid, 2-methyl-1(1,1-dimethyle	74381-40-1	0.017	0.009
44	Tetradecanoic acid	544-63-8	0.002	0.004
62	Tetradecanoic acid	544-63-8	0.055	0.037
64	Tetradecanoic acid, 12-methyl, (S)	5746-58-7	0.005	0.004
27	Undecanal	112-44-7	<0.001	--

1. CAS = Chemical Abstract Service.

2. Average of 5 TST samples; 3 were 4-L and 2 were 1-L; presented values are estimates.

Table 4-9
Tank C-108 Tentatively Identified Organic Compounds in TST Samples
Sorted by Estimated Concentration--
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
63	Benzenesulfonamide, N-butyl	3622-84-2	0.132	0.103
73	Hexadecanoic acid	57-10-3	0.120	0.088
3	Acetic Acid	64-19-7	0.083	0.117
72	9-Hexadecenoic acid	2091-29-4	0.062	0.052
62	Tetradecanoic acid	544-63-8	0.055	0.037
2	Methane, trichlorofluoro	75-69-4	0.042	0.032
4	Acetic Acid	64-19-7	0.038	0.085
1	1-Butene	106-98-9	0.038	0.053
7	Cyclotrisiloxane, hexamethyl	541-05-9	0.026	0.020
66	Pentadecanoic acid	1002-84-2	0.023	0.016
13	Cyclotetrasiloxane, octamethyl	556-67-2	0.020	0.026
20	Nonanal	124-19-6	0.018	0.024
49	Propanoic acid, 2-methyl-1(1,1-dimethyle	74381-40-1	0.017	0.009
67	C14-Alkene		0.016	0.028
15	Octanal	124-13-0	0.016	0.029
68	1-Hexadecanol	36653-82-4	0.012	0.020
8	Alkanone		0.012	0.026
23	Decanal	112-31-2	0.011	0.013
46	Dodecanoic acid	143-07-7	0.010	0.007
6	Hexanal	66-25-1	0.010	0.023
9	Heptanal	111-71-7	0.009	0.021
50	Benzenamine, N-phenyl	122-39-4	0.009	0.006
80	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.007	0.006
19	Benzenemethanol, a,a-dimethyl	617-94-7	0.006	0.002
16	1-Hexanol, 2-Ethyl	104-76-7	0.006	0.005
64	Tetradecanoic acid, 12-methyl, (S)	5746-58-7	0.005	0.004

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
10	4H-1,2,4-Triazol-3-amine, 4-ethyl	42786-06-1	0.004	0.006
71	Alkane		0.004	0.010
74	1,2-Benzenedicarboxylic acid, butyl 2-me	17851-53-5	0.004	0.006
17	1-Octanol	111-87-5	0.004	0.009
5	Propanoic acid	79-09-4	0.003	0.008
40	C12-Alkene		0.003	0.002
48	Dodecane, 2-methyl-6-propyl	55045-08-4	0.003	0.004
60	9-Octadecenoic acid, (Z)-	112-80-1	0.003	0.004
52	N-Hexyl-benzene-sulfonamide		0.003	0.003
31	Alkane		0.002	0.002
37	5,9-Undecadio-2-one, 6,10-dimethyl-, (Z)	3879-26-3	0.002	0.002
33	n-Tetradecane	629-59-4	0.002	0.003
21	Benzoic acid, 2-{trimethylsilyl}oxy]-trimeth	3789-85-3	0.002	0.002
22	1-Nonanol	143-08-8	0.002	0.003
79	Hexadecanoic acid	57-10-3	0.002	0.004
42	2,5-Cyclohexadiene-1,4-dione, 2,6-bis	719-22-2	0.002	0.002
78	1-Hexadecanol, 2-methyl	2490-48-4	0.002	0.002
44	Tetradecanoic acid	544-63-8	0.002	0.004
77	1-Hexadecanol, acetate	629-70-9	0.002	0.004
12	Cyclobutane, 1,1,2,3,3-pentamethyl	57905-86-9	0.002	0.004
59	Mixture		0.002	0.002
58	Mixture (alkane and alkanoic acid)		0.002	0.002
57	1-Hexadecanol and others		0.002	0.003
53	para-T-Butyl Benzoic acid, methyl ester		0.002	0.003
51	Hexadecanamide	629-54-9	0.001	0.001
35	Mixture		<0.001	--
36	Decane, 1,1'-oxybis	2456-28-2	<0.001	--
54	1,2-Benzenedicarboxylic acid, bis-(2ethyl	117-81-7	0.001	0.002

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	Octadecanoic acid	57-11-4	0.001	0.002
56	Mixture		0.001	0.002
18	Ethanone, 1-phenyl	98-86-2	0.001	0.001
38	2,5-Cyclohexadiene, 1,4-dione, 2,6-bis(1	719-22-2	<0.001	--
47	n-Tetradecane	629-59-4	<0.001	--
34	Dodecanal	112-54-9	<0.001	--
61	1,1'-Biphenyl, 2,2'-diethyl	13049-35-9	0.001	0.001
32	Butanoic acid, butyl ester	109-21-7	<0.001	--
30	Butanoic acid, butyl ester and siloxane	109-21-7	<0.001	--
29	Alkane		<0.001	--
65	Cyclohexanol, 1,1'-dioxybis-and others		<0.001	--
14	Benzene, (1-methylethenyl)-	98-83-9	0.001	0.002
39	Alkanol and alkyl benzene		0.001	0.002
11	Ethanol, 2-Butoxy	111-76-2	0.001	0.001
69	Alkanol		0.001	0.003
70	n-Hexadecane	544-76-3	0.001	0.002
28	Decanoic acid	334-48-5	<0.001	--
27	Undecanal	112-44-7	<0.001	--
26	2,5-Pyrrolidinedione, 1-methyl	1121-07-9	0.001	0.001
25	1,3,5,7-Tetraazatricyclo[3.3.1.1 ^{3,7}]decane	100-97-0	0.001	0.002
75	Alkanol		<0.001	--
76	1-Hexadecanol	36653-82-4	0.001	0.003
45	Decanoic acid	334-48-5	<0.001	--
43	n-Hexadecane	544-76-3	0.001	0.001
41	Alkene		<0.001	--
24	Benzenamine, N-phenyl	122-39-4	0.001	0.002

1 CAS = Chemical Abstract Service

2 Average of 5 TST samples; 3 were 4-L and 2 were 1-L; presented values are estimates.

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