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Title/Desc:

TANK 241BX104 HEADPSACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
12/1994

ENGINEERING CHANGE NOTICE

Page 1 of 21. ECN **No 625436**Proj.
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13b. Justification Details Complete rewrite which includes all vapor sampling events to date and data qualification.			
14. Distribution (include name, MSIN, and no. of copies) See attached Distribution Sheet			RELEASE STAMP OFFICIAL RELEASE BY WHC DATE SEP 28 1995 Sta 4

ENGINEERING CHANGE NOTICE

Page 2 of 2

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

625436

15. Design
Verification
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☒ No

16. Cost Impact

ENGINEERING

CONSTRUCTION

Additional

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Savings

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Savings

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17. Schedule Impact (days)

Improvement

☐

Delay

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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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20. Approvals

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Cog. Mgr. T. J. Kelley	9/23/95	QA	
QA		Safety	
Safety		Design	
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		Signature or a Control Number that tracks the Approval Signature	
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Characterization Results for Samples Collected in
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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.

8. RELEASE STAMP

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Tank 241-BX-104 Headspace Gas and Vapor Characterization Results for Samples Collected in December 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
LFL	lower flammability limit
MS	mass spectrometer
NFPA	National Fire Protection Association
NPH	normal paraffinic hydrocarbon
ORNL	Oak Ridge National Laboratory
PNL	Pacific Northwest Laboratory
ppmv	parts per million by volume, 1 ppmv = 10 ⁻⁴ vol%
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-BX-104 Headspace Gas and Vapor Characterization Results
for Samples Collected in December 1994

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank BX-104 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). Tank BX-104 was vapor sampled 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). However, current governing operating specifications for single shell waste tanks, such as tank BX-104, specify that combustible constituents be maintained at or below 20 % of the LFL (Boyles 1994).

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 BX-104 headspace characterization data presented here are from a single 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 BX-104 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 BX-104 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank BX-104 is the first tank in a 3-tank cascade with tanks BX-105 and BX-106. It is connected to tank BX-105 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long cascade line. Tanks BX-105 and BX-106 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 BX-105 or tank BX-106 may be transferred to tank BX-104 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data are available for either tanks BX-105 or BX-106 to assess their potential effect on tank BX-104.

The cascade of tanks BX-104, BX-105, and BX-106 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 1994). Changes in the concentrations of tank headspace constituents due to barometric pressure changes are consequently very slow.

2.0 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank BX-104 using the vapor sampling system (VSS) on December 30, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by *Tank 241-BX-104 Tank Characterization Plan* (the TCP), (Carpenter 1994). The tank headspace temperature was determined to be 22.8 °C. Air from the BX-104 headspace was withdrawn from a single elevation via a 8.5-m long heated sampling probe mounted in riser 1, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 60 °C. All tank air samples were collected between 11:10 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 40 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 14 trip blanks and 2 field blanks provided by the laboratories.

A general description of vapor sampling and sample analysis methods is given by Huckaby and Babad (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 (1995).

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 and are given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM canisters were prepared and analyzed by PNL (Pool et al. 1995). PNL analyses of SUMMATM canisters and sorbent traps for inorganic compounds were performed 54 and 12 days respectively, after sample collection (Ligotke 1995), which were within the 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994). PNL results were produced at PNL quality assurance impact level 2.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The ammonia concentration in the headspace of tank BX-104 was reported as 235 ppmv. Ammonia has been observed in virtually all of the passively ventilated waste tanks sampled to date, at concentrations ranging from about 3 ppmv in tank C-108 (Lucke et al. 1995), 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 235 ppmv corresponds to about 0.16 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank BX-104 was determined to be < 94 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, 94 ppmv hydrogen concentration in tank BX-104 corresponds to about 0.24 % of its LFL. At this level, hydrogen is not a flammability concern in tank BX-104.

The nitrous oxide concentration in tank BX-104 headspace was measured at 143 ppmv. 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 878 ppmv in 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 BX-104 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

The concentration of carbon monoxide in the tank BX-104 headspace was reported as < 12 ppmv. In ambient air it typically ranges from 0.05 to 0.15 ppmv. Because different analytical methods have been used to measure carbon monoxide in the waste tanks sampled to date, the information on carbon monoxide has varied from tank to tank. However, elevated waste tank headspace carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks.

The average carbon dioxide concentration in the tank BX-104 headspace, 74 ppmv, is significantly lower than it is in ambient air. 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

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

waste tanks, and converted to carbonate in solution. The 74 ppmv of carbon dioxide measured in tank BX-104 is typical for the waste tanks sampled to date.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank BX-104 headspace were determined to be 0.3 ppmv and ≤ 0.03 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank BX-104. 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 BX-104 headspace.

The water vapor concentration of tank BX-104 was determined to be about 5.9 mg/L, at the measured tank headspace temperature of 22.8 °C and pressure of 1006 mbar (754.6 torr), (WHC 1995). This corresponds to a water vapor partial pressure of 8.1 mbar (6.1 torr), to a dew point of 4.0 °C, and to a relative humidity of 29 %.

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

3.4 Discussion of Inorganic Gases and Vapors

Aside from water and carbon dioxide, the most abundant waste constituents in the tank BX-104 headspace are ammonia and nitrous oxide. These have been detected in most tank headspaces sampled to date, and along with hydrogen, are usually the dominate waste species. The concentrations of these vapors in tank BX-104 are typical of other passively ventilated tanks that have been sampled.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are generally good for the methods and at the measured concentrations. Relative standard deviations range from about 1 % for ammonia to 36 % for carbon dioxide results. 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.), small 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 BX-104 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) to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Pool et al. (1995).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank BX-104. PNL results were produced at PNL quality assurance impact level 2. All PNL analyses were completed 20 days after sample collection. 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 included the 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 tank C-103.

Table 4-1 lists the organic compounds positively identified and quantitated in SUMMA™ samples. SUMMA™ analyses were performed according to the TO-14 methodology, except for methane analysis, which was analyzed with the inorganic gases (Pool et al. 1995). Only 3 of the 40 TO-14 target analytes (trichlorofluoromethane, benzene, and toluene) and 10 of the 14 additional target analytes were measured to be above the 0.005 ppmv detection limit of the analyses. Averages reported are from analyses of 3 SUMMA™ canister samples.

Jenkins et al. (1995a) report the positive identification of 23 of 27 target analytes in TST samples. 1,1-Dichloroethene, dichloromethane, dibutyl butylphosphonate, and tributyl phosphate were the only TST target analytes not detected. The average concentrations of the 12 positively identified and quantitated target analytes, from the analysis of 3 TSTs, are given in Table 4-2. Table 4-3 lists 8 compounds for which were outside the instrumental calibration range in at least 1 TST sample, and were consequently not quantitated. Table 4-3 lists the 3 compounds which exceeded their ORNL practical holding times. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so that no analyte appears in more than 1 of these tables.

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, of butanal, 1-butanol, and 2-pentanone exceeded their practical holding times, and may have been affected by the 38 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 of butanal, 1-butanol, and 2-pentanone are 1, 17, and 34 days, respectively. 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 SUMMATM analyses. Table 4-5 lists these, and their reported average concentrations in TST and SUMMATM samples. As indicated in Table 4-5, the reported concentrations of ethanenitrile, propanenitrile, n-butanenitrile, benzene, toluene, n-hexane, and n-decane are each significantly higher in TST samples than in SUMMATM samples.

The most abundant analytes in Tables 4-1 through 4-4 are 1-butanol, n-tridecane, propanone, and n-dodecane, each of which was measured to be above 1 ppmv. At the reported concentrations, the target analytes do not individually or collectively represent a flammability hazard.

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. 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 SUMMATM 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 SUMMATM samples has been problematic.

The list of tentatively identified compounds recovered from SUMMATM samples, with estimated concentrations, is given in Table 4-6. Compounds are listed in Table 4-6 in the order by which they eluted chromatographically, and only non-zero results are included in the reported averages. Because the list of tentatively identified organic compounds in SUMMATM samples is rather long and locating any given compound may be difficult, these compounds have been sorted alphanumerically by compound name in Table 4-7, and also in order of decreasing estimated concentrations in Table 4-8. Numbers in the first

columns of Tables 4-7 and 4-8 (Cmpd #) identify the location of the compounds in Table 4-6. Estimated concentrations are in mg/m^3 , based on dry air at 0 °C and 1.01 bar.

The list of tentatively identified compounds detected in TST samples and their estimated concentrations is given in Table 4-9. Compounds are listed in Table 4-9 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table 4-9 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/m^3 , based on dry air at 0 °C and 1.01 bar.

As with the SUMMATM results, the list of compounds tentatively identified in TSTs has been sorted alphanumerically in Table 4-10, and also in order of decreasing estimated concentrations in Table 4-11. Numbers in the first columns of Tables 4-10 and 4-11 (Cmpd #) identify the location of the compounds in Table 4-9.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and Pool et al. (1995), respectively, and should be reviewed before this data are used for decision making. The quantitative measurement 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 and 4-9 should be considered rough estimates. Results in Tables 4-6 and 4-9 are presented in terms of observed chromatographic peaks, and are not adjusted for the occurrence of split peaks or the assignment of the same identity to different peaks (e.g., Cmpd # 34 and 55 in Table 4-9). In these instances, the estimated concentration of a compound appearing in more than 1 peak is simply the sum of the individual peak estimates.

4.3 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables 4-1 through 4-9 is to separate them into 2 categories: 1) Organic compounds added to tank BX-104 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 tentatively identified alkyl-substituted decahydronaphthalenes, and semivolatile branched and straight-chain alkanes, which were used as diluents of tributyl phosphate in various plutonium extraction processes. The semivolatile straight-chain alkanes (i.e., n-undecane, n-dodecane, n-tridecane, n-tetradecane, and n-pentadecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs).

The tentatively identified cyclosiloxanes (i.e., Cmpd # 9 and 16 in Table 4-9) may also be 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.

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 4-11 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. While both larger and smaller molecules are

generated from the waste, the most abundant of these in the headspace are the smaller, short-chain volatile compounds.

The notable absence of tributyl phosphate in the tank BX-104 samples may be due to a sampling difficulty. The abundance of the tributyl phosphate diluents and their degradation products is reason to expect tributyl phosphate to be present in the tank waste. 1-Butanol, which had the highest reported concentration of compounds in TST samples and the third highest concentration of organic compounds in SUMMA™ samples, is known to be a product of the hydrolysis of tributyl phosphate. Furthermore, informal tests by ORNL indicate that tributyl phosphate is adsorbed by the glass fiber filters used during sampling to protect the samples from radiolytic particulate contamination. Based on these considerations, the concentration of tributyl phosphate in the tank BX-104 headspace should be considered to be unknown.

The total organic vapor concentration of tank BX-104 was estimated by Jenkins et al.(1995a) to be about 100 mg/m³ from the analysis of a single TST sample by GC with flame ionization detection. A summation of concentrations of positively and tentatively identified compounds in 3 TST samples by GC/MS indicated the total organic vapor concentration to be about 85 mg/m³.

Jenkins et al. (1995a) reported that propanone, n-dodecane, and n-tridecane were detected in the trip and field TST blanks at trace levels. The concentrations of these analytes in the TST blanks were less than 1 % of their concentrations in tank BX-104 samples. Dichloromethane was also detected in the TST blanks, but not in the tank BX-104 samples. Jenkins et al (1995a). also report that benzene and toluene were detected in the TST field blanks, at levels less than half of the tank samples.

Ambient air SUMMA™ samples collected during the tank BX-104 sampling event suggest the VSS manifold may have been contaminated with trace amounts of acetone. Specifically, analysis of an ambient air sample collect upwind of the VSS (not through the VSS manifold) indicated acetone to be present at < 0.005 ppmv, while an ambient air sample collected through the VSS (to check system cleanliness) was determined to have about 0.012 ppmv of acetone. Residual amounts of acetone, used as a cleaning solvent, may have been present in the VSS transfer tubing.

In summary, the organic vapor concentrations in tank BX-104 are relatively high. The organic vapors in tank BX-104 clearly indicate the presence of the semivolatile NPHs and their degradation products in the tank waste. Though tributyl phosphate was not detected in any of the headspace samples, there is strong evidence that it is also present in the waste.

5.0 SUMMARY

The tank BX-104 headspace was sampled in December 1994 for gases and vapors to address flammability and industrial hygiene concerns. Results unique to the sampling event and essentially all results have been reported. It was determined that no headspace constituents exceeded the flammability notification limits, but that ammonia, measured to be 235 ppmv, exceeded the 150 ppmv industrial hygiene notification limit specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

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Table 2-1
Tank BX-104 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	0.2	Organic vapors	4 tank air samples
		1.0	Organic vapors	4 tank air samples
		4.0	Organic vapors	4 tank air samples
				+ 2 trip blanks + 2 field blanks
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blank
	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, Methane, 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 BX-104 Inorganic Gas and Vapor Concentrations

Compound	CAS ¹ Number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	235	3	1
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	74	27	36
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	< 12	—	—
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	< 94	—	—
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.3	0.02	7
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.03	—	—
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	143	7	5
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	8,100 (5.9 mg/L)	400 (0.3 mg/L)	4.7

¹ CAS = Chemical Abstracts Service.

² RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

Table 4-1
Tank BX-104 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	Propanenitrile (acetonitrile) ⁴	75-05-8	0.052	—	—
2	Propanone (acetone)	67-64-1	1.40	0.37	26
3	Trichlorofluoromethane	75-69-4	0.14	0.042	30
4	Propanol	71-23-8	0.32	0.098	30
5	2-Butanone	78-93-3	0.22	0.010	4
6	Tetrahydrofuran	109-99-9	0.36	0.19	5
7	n-Butanenitrile	109-74-0	0.020	0.005	24
8	Benzene	71-43-2	0.005	0.0003	6
9	n-Heptane	142-82-5	0.067	0.001	2
10	4-Methyl-2-Pentanone	108-10-1	0.011	0.0003	3
11	Pyridine	110-86-1	0.089	0.028	31
12	Toluene	108-88-3	0.0070	0.0002	3
13	n-Decane ⁴	124-18-5	0.012	—	—
14	Methane	74-82-8	< 61	—	—

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 This compound was only detected in 1 sample.

Table 4-2
Tank BX-104 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	Ethanenitrile (acetonitrile)	75-05-8	0.34	0.02	5
2	Propanenitrile	107-12-0	0.070	0.004	5
3	n-Hexane	110-54-3	0.16	0.02	11
4	n-Butanenitrile	109-74-0	0.059	0.005	8
5	n-Heptane	142-82-5	0.067	0.011	17
6	2-Hexanone	591-78-6	0.059	0.005	8
7	n-Octane	111-65-9	0.043	0.002	5
8	2-Heptanone	110-43-0	0.093	0.009	10
9	n-Nonane	111-84-2	0.039	0.003	9
10	2-Octanone	111-13-7	0.043	0.006	13
11	n-Decane	124-18-5	0.037	0.003	7
12	n-Undecane	1120-21-4	0.26	0.01	5

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 200 ml TST samples.

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

Table 4-3
Tank BX-104 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	Propanone (acetone)	67-64-1	1.22	0.07	5
2	Benzene	71-43-2	0.011	0.001	5
3	Toluene	108-88-3	0.013	0.001	7
4	n-Pentanenitrile	110-59-8	0.023	0.002	7
5	n-Hexanenitrile	628-73-9	0.020	0.002	11
6	n-Heptanenitrile	629-08-3	0.023	0.003	11
7	n-Dodecane	112-40-3	1.12	0.14	12
8	n-Tridecane	629-50-5	2.01	0.28	14

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, 200 ml TST samples.

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

Table 4-4
Tank BX-104 Positively Identified Organic 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	Butanal ⁵	123-72-8	0.36	0.13	36
2	1-Butanol ⁶	71-36-3	4.62	0.41	9
3	2-Pentanone ⁵	107-87-9	0.12	0.01	11

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 200 ml TST samples.

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

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

6 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 BX-104 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	< 0.012	< 0.005	--
Dichloromethane (methylene chloride)	75-09-2	< 0.027	< 0.005	--
Propanone (acetone)	67-64-1	1.22	1.4	137
Ethanenitrile (acetonitrile)	75-05-8	0.34	0.052	147
Propanenitrile	107-12-0	0.070	< 0.005	> 173
n-Butanenitrile	109-74-0	0.059	0.020	99
Benzene	71-43-2	0.011	0.005	75
Toluene	108-88-3	0.013	0.0070	60
n-Hexane	110-54-3	0.16	< 0.005	> 188
n-Heptane	142-82-5	0.067	0.067	0
n-Decane	124-18-5	0.037	0.012	102

1 CAS = Chemical Abstract Service.

2 Average of 3, 200 ml TST samples by ORNL.

3 Average of 3 samples by PNL.

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

Table 4-6
 Tank BX-104 Tentatively Identified Organic Compounds in SUMMA™ Samples
 in Order of Chromatographic Elution --
 Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
1	Propene	115-07-1	0.35	0.17
2	Propane	74-98-6	0.32	0.03
3	Methyl nitrite	624-91-9	0.13	0.02
4	Cyclopropane	75-19-4	0.13	0.01
5	Isobutane	75-28-5	0.074	0.007
6	Methanol	67-56-1	0.40	0.04
7	1-Butene	106-98-9	0.12	0.01
8	n-Butane	106-97-8	0.41	0.04
9	2-Methylpropene	115-11-7	0.077	0.008
10	Ethanol	64-17-5	0.16	0.04
11	1-Pentene ⁴	109-67-1	0.06	—
12	n-Pentane	109-66-0	0.28	0.05
13	2-Methylpentane	107-83-5	0.24	0.01
14	Butanal	123-72-8	0.42	0.08
15	2-Butanol	78-92-2	0.076	0.002
16	1-Butanol	71-36-3	5.76	0.79
17	2-Pentanone	107-87-9	0.29	0.02
18	Unknown alkyl nitrile		0.22	0.06
19	1-Pentanol	71-41-0	0.078	0.012
20	2,5-Dimethylhexane	592-13-2	0.076	0.002
21	2-Hexanone	591-78-6	0.15	0.002
22	Hexanal ⁴	66-25-1	0.08	—
23	Butyl nitrate	928-45-0	0.29	0.01
24	5-Methyl-2-hexanone ⁵	110-12-3	0.05	< 0.01
25	1-Hexanol	111-27-3	0.091	0.007
26	3-Heptanone	106-35-4	0.36	0.02
27	2-Heptanone	10-43-0	0.19	0.01

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
28	n-Butyl ether ⁴	142-96-1	0.05	--
29	3-Heptanol ⁴	589-82-2	0.11	--
30	n-Nonane	111-84-2	0.12	0.01
31	Pentyl nitrate	1002-16-0	0.054	0.006
32	6-Methyl-2-heptanone	928-68-7	0.35	0.03
33	Heptanenitrile	629-08-3	0.065	0.008
34	1-Heptanol ⁴	111-70-6	0.05	--
35	2-Octanone	111-13-7	0.11	0.01
36	2-Ethyl-1-hexanol	104-76-7	0.066	0.023
37	4-Methyldecane	2847-72-5	0.061	0.006
38	Unknown alkyl nitrate		0.12	0.01
39	Unknown C9 ketone		0.094	0.012
40	Octanenitrile	124-12-9	0.059	0.009
41	2-Nonanone	21-55-6	0.074	0.012
42	n-Undecane	1120-21-4	1.61	0.18
43	Unknown C12 alkane		< 0.08	--
44	5-Methylundecane	1632-70-8	0.068	0.005
45	Pentylcyclohexane	4292-92-6	0.056	0.005
46	2,5-Dimethyldecane	17312-50-4	0.17	0.06
47	4-Methylundecane	2980-69-0	0.071	0.016
48	2-Methylundecane	7045-71-8	0.20	0.02
49	3-Methylundecane	1002-43-3	0.12	0.01
50	2-Decanone ⁴	693-54-9	0.06	--
51	Unknown alkane		0.14	0.05
52	n-Dodecane	112-40-3	6.92	0.95
53	Decahydro-2,6-dimethylnaphthalene	1618-22-0	0.12	0.02
54	Unknown C13 alkane		1.72	0.23
55	Unknown C13 alkane		0.20	0.02
56	Unknown alkyl decahydronaphthalene ⁵		0.22	0.005

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
57	Unknown C13 alkene/Cycloalkane		1.03	0.12
58	Unknown C13 alkane		0.35	0.03
59	Unknown C13 alkane		0.43	0.04
60	Unknown C13 alkane		0.33	0.03
61	7-Methyltridecane	26730-14-3	2.68	0.26
62	Unknown C8 cyclohexane		0.21	0.02
63	n-Tridecane	629-50-5	8.11	0.86
64	Unknown C8 cyclohexane		0.45	0.06
65	Unknown C14 alkane		0.54	0.06
66	Unknown C13 alkene/Cycloalkane ⁵		0.21	0.09
67	Unknown C7 cyclohexane ⁵		0.31	0.015
68	2-Methyltridecane	1560-96-9	0.12	0.02
69	3-Methyltridecane ⁴	6418-41-3	0.09	—
70	Unknown C15 alkane		0.60	0.08
71	Unknown C4 decahydronaphthalene ⁵		0.19	0.005
72	n-Tetradecane	629-59-4	0.75	0.15
73	Unknown C15 alkene/ Cycloalkane ⁴		0.16	—
74	Unknown C9 cyclohexane ⁵		0.16	0.01
Sum of tentatively identified compounds:			39.99	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples by PNL, values listed are estimates.

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 1 sample.

5 Detected in only 2 samples.

Table 4-7
 Tank BX-104 Tentatively Identified Organic Compounds in SUMMA™ Samples
 Sorted Alphanumerically –
 Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
34	1-Heptanol ³	111-70-6	0.05	—
11	1-Pentene ⁴	109-67-1	0.06	—
16	1-Butanol	71-36-3	5.76	0.79
25	1-Hexanol	111-27-3	0.091	0.007
19	1-Pentanol	71-41-0	0.078	0.012
7	1-Butene	106-98-9	0.12	0.01
48	2-Methylundecane	7045-71-8	0.20	0.02
35	2-Octanone	111-13-7	0.11	0.01
9	2-Methylpropene	115-11-7	0.077	0.008
50	2-Decanone ⁴	693-54-9	0.06	—
27	2-Heptanone	10-43-0	0.19	0.01
36	2-Ethyl-1-hexanol	104-76-7	0.066	0.023
13	2-Methylpentane	107-83-5	0.24	0.01
68	2-Methyltridecane	1560-96-9	0.12	0.02
15	2-Butanol	78-92-2	0.076	0.002
21	2-Hexanone	591-78-6	0.15	0.002
17	2-Pentanone	107-87-9	0.29	0.02
41	2-Nonanone	21-55-6	0.074	0.012
46	2,5-Dimethyldecane	17312-50-4	0.17	0.06
20	2,5-Dimethylhexane	592-13-2	0.076	0.002
49	3-Methylundecane	1002-43-3	0.12	0.01
69	3-Methyltridecane ⁴	6418-41-3	0.09	—
29	3-Heptanol ⁴	589-82-2	0.11	—
26	3-Heptanone	106-35-4	0.36	0.02
47	4-Methylundecane	2980-69-0	0.071	0.016
37	4-Methyldecane	2847-72-5	0.061	0.006
24	5-Methyl-2-hexanone ⁵	110-12-3	0.05	< 0.01

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
44	5-Methylundecane	1632-70-8	0.068	0.005
32	6-Methyl-2-heptanone	928-68-7	0.35	0.03
61	7-Methyltridecane	26730-14-3	2.68	0.26
14	Butanal	123-72-8	0.42	0.08
23	Butyl nitrate	928-45-0	0.29	0.01
4	Cyclopropane	75-19-4	0.13	0.01
53	Decahydro-2,6-dimethylnaphthalene	1618-22-0	0.12	0.02
10	Ethanol	64-17-5	0.16	0.04
33	Heptanenitrile	629-08-3	0.065	0.008
22	Hexanal ⁴	66-25-1	0.08	--
5	Isobutane	75-28-5	0.074	0.007
6	Methanol	67-56-1	0.40	0.04
3	Methyl nitrite	624-91-9	0.13	0.02
28	n-Butyl ether ⁴	142-96-1	0.05	--
8	n-Butane	106-97-8	0.41	0.04
52	n-Dodecane	112-40-3	6.92	0.95
30	n-Nonane	111-84-2	0.12	0.01
12	n-Pentane	109-66-0	0.28	0.05
72	n-Tetradecane	629-59-4	0.75	0.15
63	n-Tridecane	629-50-5	8.11	0.86
42	n-Undecane	1120-21-4	1.61	0.18
40	Octanenitrile	124-12-9	0.059	0.009
31	Pentyl nitrate	1002-16-0	0.054	0.006
45	Pentylcyclohexane	4292-92-6	0.056	0.005
2	Propane	74-98-6	0.32	0.03
1	Propene	115-07-1	0.35	0.17
18	Unknown alkyl nitrile		0.22	0.06
38	Unknown alkyl nitrate		0.12	0.01
39	Unknown C9 ketone		0.094	0.012

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
43	Unknown C12 alkane		< 0.08	--
51	Unknown alkane		0.14	0.05
54	Unknown C13 alkane		1.72	0.23
55	Unknown C13 alkane		0.20	0.02
56	Unknown alkyl decahydronaphthalene ⁵		0.22	0.005
57	Unknown C13 alkene/Cycloalkane		1.03	0.12
58	Unknown C13 alkane		0.35	0.03
59	Unknown C13 alkane		0.43	0.04
60	Unknown C13 alkane		0.33	0.03
62	Unknown C8 cyclohexane		0.21	0.02
64	Unknown C8 cyclohexane		0.45	0.06
65	Unknown C14 alkane		0.54	0.06
66	Unknown C13 alkene/Cycloalkane ⁵		0.21	0.09
67	Unknown C7 cyclohexane ⁵		0.31	0.015
70	Unknown C15 alkane		0.60	0.08
71	Unknown C4 decahydronaphthalene ⁵		0.19	0.005
73	Unknown C15 alkene/Cycloalkane ⁴		0.16	--
74	Unknown C9 cyclohexane ⁵		0.16	0.01
Sum of tentatively identified compounds:			39.99	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples by PNL; values listed are estimates.

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 1 sample.

5 Detected in only 2 samples.

Table 4-8
 Tank BX-104 Tentatively Identified Organic Compounds in SUMMA™ Samples
 Sorted by Estimated Concentration --
 Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
63	n-Tridecane	629-50-5	8.11	0.86
52	n-Dodecane	112-40-3	6.92	0.95
16	1-Butanol	71-36-3	5.76	0.79
61	7-Methyltridecane	26730-14-3	2.68	0.26
42	n-Undecane	1120-21-4	1.61	0.18
72	n-Tetradecane	629-59-4	0.75	0.15
14	Butanal	123-72-8	0.42	0.08
8	n-Butane	106-97-8	0.41	0.04
6	Methanol	67-56-1	0.40	0.04
26	3-Heptanone	106-35-4	0.36	0.02
1	Propene	115-07-1	0.35	0.17
32	6-Methyl-2-heptanone	928-68-7	0.35	0.03
2	Propane	74-98-6	0.32	0.03
17	2-Pentanone	107-87-9	0.29	0.02
23	Butyl nitrate	928-45-0	0.29	0.01
12	n-Pentane	109-66-0	0.28	0.05
13	2-Methylpentane	107-83-5	0.24	0.01
54	Unknown C13 alkane		1.72	0.23
48	2-Methylundecane	7045-71-8	0.20	0.02
27	2-Heptanone	10-43-0	0.19	0.01
46	2,5-Dimethyldecane	17312-50-4	0.17	0.06
10	Ethanol	64-17-5	0.16	0.04
21	2-Hexanone	591-78-6	0.15	0.002
3	Methyl nitrite	624-91-9	0.13	0.02
4	Cyclopropane	75-19-4	0.13	0.01
7	1-Butene	106-98-9	0.12	0.01
68	2-Methyltridecane	1560-96-9	0.12	0.02

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
49	3-Methylundecane	1002-43-3	0.12	0.01
57	Unknown C13 alkene/Cycloalkane		1.03	0.12
53	Decahydro-2,6-dimethylnaphthalene	1618-22-0	0.12	0.02
30	n-Nonane	111-84-2	0.12	0.01
29	3-Heptanol ⁴	589-82-2	0.11	—
35	2-Octanone	111-13-7	0.11	0.01
25	1-Hexanol	111-27-3	0.091	0.007
66	Unknown C13 alkene/Cycloalkane ⁵		0.21	0.09
69	3-Methyltridecane ⁴	6418-41-3	0.09	—
22	Hexanal ⁴	66-25-1	0.08	—
70	Unknown C15 alkane		0.60	0.08
19	1-Pentanol	71-41-0	0.078	0.012
9	2-Methylpropene	115-11-7	0.077	0.008
20	2,5-Dimethylhexane	592-13-2	0.076	0.002
15	2-Butanol	78-92-2	0.076	0.002
41	2-Nonanone	21-55-6	0.074	0.012
5	Isobutane	75-28-5	0.074	0.007
47	4-Methylundecane	2980-69-0	0.071	0.016
44	5-Methylundecane	1632-70-8	0.068	0.005
36	2-Ethyl-1-hexanol	104-76-7	0.066	0.023
33	Heptanenitrile	629-08-3	0.065	0.008
37	4-Methyldecane	2847-72-5	0.061	0.006
50	2-Decanone ⁴	693-54-9	0.06	—
65	Unknown C14 alkane		0.54	0.06
64	Unknown C8 cyclohexane		0.45	0.06
11	1-Pentene ⁴	109-67-1	0.06	—
18	Unknown alkyl nitrile		0.22	0.06
40	Octanenitrile	124-12-9	0.059	0.009
45	Pentylcyclohexane	4292-92-6	0.056	0.005

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
31	Pentyl nitrate	1002-16-0	0.054	0.006
51	Unknown alkane		0.14	0.05
24	5-Methyl-2-hexanone ⁵	110-12-3	0.05	< 0.01
28	n-Butyl ether ⁴	142-96-1	0.05	—
34	1-Heptanol ⁴	111-70-6	0.05	—
59	Unknown C13 alkane		0.43	0.04
58	Unknown C13 alkane		0.35	0.03
60	Unknown C13 alkane		0.33	0.03
55	Unknown C13 alkane		0.20	0.02
62	Unknown C8 cyclohexane		0.21	0.02
67	Unknown C7 cyclohexane ⁵		0.31	0.015
39	Unknown C9 ketone		0.094	0.012
74	Unknown C9 cyclohexane ⁵		0.16	0.01
38	Unknown alkyl nitrate		0.12	0.01
56	Unknown alkyl decahydronaphthalene ⁵		0.22	0.005
71	Unknown C4 decahydro-naphthalene ⁵		0.19	0.005
43	Unknown C12 alkane		< 0.08	—
73	Unknown C15 alkene/Cycloalkane ⁴		0.16	—
Sum of tentatively identified compounds:			39.99	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples by PNL, values listed are estimates.

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 1 sample.

5 Detected in only two samples.

Table 4-9
Tank BX-104 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	n-Butane	106-97-8	0.80	0.16
2	Ethanol and butane, 2-methyl-		0.20	0.18
3	1-Propanol	71-23-8	0.48	0.02
4	2-Butanone	78-93-3	0.26	0.01
5	Nitrous acid, butyl ester	544-16-1	0.062	0.110
6	Furan, tetrahydro-	109-99-9	0.55	0.07
7	1H-Pyrazole, 3-methyl-	1453-58-3	0.23	0.05
8	1-Pentanol	71-41-0	0.062	0.110
9	Cyclotrisiloxane, hexamethyl-	541-05-9	0.48	0.16
10	Nitric acid, butyl ester	928-45-0	0.17	0.01
11	1-Hexanol	111-27-3	0.17	0.03
12	3-Heptanone	106-35-4	0.54	0.05
13	Nitric acid, pentyl ester	1002-16-0	0.049	0.085
14	2-Heptanone, 6-methyl-	928-68-7	0.59	0.08
15	1-Heptanol	111-70-6	0.052	0.090
16	Cyclotetrasiloxane, octamethyl-	556-67-2	0.21	0.20
17	1-Hexanol, 2-ethyl-	104-76-7	0.23	0.04
18	Oxirane, 2-ethyl-3-propyl-, cis-	56052-94-9	0.16	0.02
19	2-Heptanone, 6-methyl-	928-68-7	0.15	0.02
20	1-Octanol	111-87-5	0.17	0.02
21	2-Nonanone	821-55-6	0.046	0.080
22	Octane, 6-ethyl-2-methyl-	62016-19-7	0.17	0.02
23	Cyclohexane, pentyl-	4292-92-6	0.13	0.11
24	Naphthalene, decahydro-2-methyl	2958-76-1	0.037	0.064
25	Undecane, 6-methyl-	17302-33-9	0.36	0.05
26	Undecane, 4-methyl-	2980-69-0	0.21	0.02

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	Undecane, 2-methyl-	7045-71-8	0.41	0.05
28	Decane, 3,8-dimethyl-	17312-55-9	0.30	0.04
29	Decane, 2,4,6-trimethyl-	62108-27-4	0.20	0.02
30	Cyclohexane, 1-ethyl-4-methyl-, cis-	4926-78-7	0.57	0.06
31	Naphthalene, decahydro-2, 6-dimethyl-	1618-22-0	0.039	0.068
32	4-Undecene, 6-methyl		0.24	0.01
33	Undecane, 2,6-dimethyl-	17301-23-4	2.17	0.19
34	Dodecane, 3-methyl-	17312-57-1	0.46	0.05
35	Decane, 2,3,7-trimethyl-	62238-13-5	0.16	0.02
36	Cyclododecane	294-62-2	0.16	0.01
37	Naphthalene, decahydro-2, 3-dimethyl-	1008-80-6	0.039	0.068
38	4-Nonene, 5-butyl-	7367-38-6	0.085	0.074
39	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.84	0.09
40	C6-Cyclohexane		1.77	0.16
41	Undecane, 2,3-dimethyl-	17312-77-5	0.78	0.11
42	Decane, 2,3,7-trimethyl-	62238-13-5	0.85	0.11
43	Cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.31	0.02
44	Octane, 2,3,7-trimethyl-	62016-34-6	3.05	0.32
45	Cyclohexane, 1,1,3,5-tetramethyl-	50876-32-9	0.15	0.27
46	2(3H)-Benzofuranone, 3a, 4,5,6- tetrahydro-trimethyl-	16778-26-0	0.30	0.03
47	3-Undecanone	2216-87-7	0.30	0.11
48	Tridecane, 7-methyl-	26730-14-3	0.26	0.02
49	Undecane, 5,5-dimethyl-	17312-73-1	1.42	0.14
50	C3-Decahydronaphthalene		0.24	0.03
51	Cyclohexane, 1,3,5-trimethyl-2-octadecyl-	55282-34-3	0.048	0.084
52	Dodecane, 2,5-dimethyl-	56292-65-0	0.061	0.100
53	C7-Cyclohexane		1.07	0.07
54	Tridecane, 2-methyl-	1560-96-9	0.48	0.04

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	Dodecane, 3-methyl-	17312-57-1	0.54	0.06
56	Tetradecane, 4-methyl-	25117-24-2	3.13	0.33
57	1,1'-Bicyclohexyl, 2-methyl-, cis-	50991-08-7	0.12	0.02
58	3-Dodecanone	1534-27-6	0.31	0.05
59	Tetradecane	629-59-4	3.61	0.57
60	Tridecane, 4,8-dimethyl-	55030-62-1	0.57	0.09
61	Cyclohexane, 1,1,3-trimethyl- 2-(3-methylpentyl)-	54965-05-8	0.74	0.09
62	Hexadecane	544-76-3	0.55	0.10
63	6-Tridecanone	22026-12-6	0.31	0.07
64	3-Tridecanone	1534-26-5	0.17	0.06
65	Pentadecane	629-62-9	0.16	0.02
66	Benzenesulfonamide, N-butyl-	3622-84-2	0.097	0.088
Sum of tentatively identified compounds:			33.63	

¹ CAS = Chemical Abstract Service.

² Average of 3, 200 ml TST samples by ORNL, values listed are estimates.

Table 4-10
 Tank BX-104 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)
3	1-Propanol	71-23-8	0.48	0.02
20	1-Octanol	111-87-5	0.17	0.02
11	1-Hexanol	111-27-3	0.17	0.03
8	1-Pentanol	71-41-0	0.062	0.110
15	1-Heptanol	111-70-6	0.052	0.090
17	1-Hexanol, 2-ethyl-	104-76-7	0.23	0.04
57	1,1'-Bicyclohexyl, 2-methyl-, cis-	50991-08-7	0.12	0.02
7	1H-Pyrazole, 3-methyl-	1453-58-3	0.23	0.05
14	2-Heptanone, 6-methyl-	928-68-7	0.59	0.08
21	2-Nonanone	821-55-6	0.046	0.080
19	2-Heptanone, 6-methyl-	928-68-7	0.15	0.02
4	2-Butanone	78-93-3	0.26	0.01
46	2(3H)-Benzofuranone, 3a,4,5,6-tetrahydro-trimethyl-	16778-26-0	0.30	0.03
47	3-Undecanone	2216-87-7	0.30	0.11
58	3-Dodecanone	1534-27-6	0.31	0.05
12	3-Heptanone	106-35-4	0.54	0.05
64	3-Tridecanone	1534-26-5	0.17	0.06
32	4-Undecene, 6-methyl-		0.24	0.01
38	4-Nonene, 5-butyl-	7367-38-6	0.085	0.074
63	6-Tridecanone	22026-12-6	0.31	0.07
66	Benzenesulfonamide, N-butyl-	3622-84-2	0.097	0.088
50	C3-Decahydronaphthalene		0.24	0.03
40	C6-Cyclohexane		1.77	0.16
53	C7-Cyclohexane		1.07	0.07
36	Cyclododecane	294-62-2	0.16	0.01
23	Cyclohexane, pentyl-	4292-92-6	0.13	0.11

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
45	Cyclohexane, 1,1,3,5-tetramethyl-	50876-32-9	0.15	0.27
43	Cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.31	0.02
30	Cyclohexane, 1-ethyl-4-methyl-, cis-	4926-78-7	0.57	0.06
61	Cyclohexane, 1,1,3-trimethyl-2-(3-methylpentyl)-	54965-05-8	0.74	0.09
39	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.84	0.09
51	Cyclohexane, 1,3,5-trimethyl-2-octadecyl-	55282-34-3	0.048	0.084
16	Cyclotetrasiloxane, octamethyl-	556-67-2	0.21	0.20
9	Cyclotrisiloxane, hexamethyl-	541-05-9	0.48	0.16
35	Decane, 2,3,7-trimethyl-	62238-13-5	0.16	0.02
29	Decane, 2,4,6-trimethyl-	62108-27-4	0.20	0.02
28	Decane, 3,8-dimethyl-	17312-55-9	0.30	0.04
42	Decane, 2,3,7-trimethyl-	62238-13-5	0.85	0.11
52	Dodecane, 2,5-dimethyl-	56292-65-0	0.061	0.100
34	Dodecane, 3-methyl-	17312-57-1	0.46	0.05
55	Dodecane, 3-methyl-	17312-57-1	0.54	0.06
2	Ethanol and butane, 2-methyl-		0.20	0.18
6	Furan, tetrahydro-	109-99-9	0.55	0.07
62	Hexadecane	544-76-3	0.55	0.10
1	n-Butane	106-97-8	0.80	0.16
24	Naphthalene, decahydro-2-methyl-	2958-76-1	0.037	0.064
37	Naphthalene, decahydro-2, 3-dimethyl-	1008-80-6	0.039	0.068
31	Naphthalene, decahydro-2, 6-dimethyl-	1618-22-0	0.039	0.068
13	Nitric acid, pentyl ester	1002-16-0	0.049	0.085
10	Nitric acid, butyl ester	928-45-0	0.17	0.01
5	Nitrous acid, butyl ester	544-16-1	0.062	0.110
22	Octane, 6-ethyl-2-methyl-	62016-19-7	0.17	0.02
44	Octane, 2,3,7-trimethyl-	62016-34-6	3.05	0.32
18	Oxirane, 2-ethyl-3-propyl-, cis-	56052-94-9	0.16	0.02

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
65	Pentadecane	629-62-9	0.16	0.02
56	Tetradecane, 4-methyl-	25117-24-2	3.13	0.33
59	Tetradecane	629-59-4	3.61	0.57
48	Tridecane, 7-methyl-	26730-14-3	0.26	0.02
54	Tridecane, 2-methyl-	1560-96-9	0.48	0.04
60	Tridecane, 4,8-dimethyl-	55030-62-1	0.57	0.09
26	Undecane, 4-methyl-	2980-69-0	0.21	0.02
25	Undecane, 6-methyl-	17302-33-9	0.36	0.05
27	Undecane, 2-methyl-	7045-71-8	0.41	0.05
41	Undecane, 2,3-dimethyl-	17312-77-5	0.78	0.11
49	Undecane, 5,5-dimethyl-	17312-73-1	1.42	0.14
33	Undecane, 2,6-dimethyl-	17301-23-4	2.17	0.19
Sum of tentatively identified compounds:			33.63	

1 CAS = Chemical Abstract Service.

2 Average of 3, 200 ml TST samples by ORNL, values listed are estimates.

Table 4-11
 Tank BX-104 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)
59	Tetradecane	629-59-4	3.61	0.57
56	Tetradecane, 4-methyl-	25117-24-2	3.13	0.33
44	Octane, 2,3,7-trimethyl-	62016-34-6	3.05	0.32
33	Undecane, 2,6-dimethyl-	17301-23-4	2.17	0.19
40	C6-Cyclohexane		1.77	0.16
49	Undecane, 5,5-dimethyl-	17312-73-1	1.42	0.14
53	C7-Cyclohexane		1.07	0.07
42	Decane, 2,3,7-trimethyl-	62238-13-5	0.85	0.11
39	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.84	0.09
1	n-Butane	106-97-8	0.80	0.16
41	Undecane, 2,3-dimethyl-	17312-77-5	0.78	0.11
61	Cyclohexane, 1,1,3-trimethyl- 2-(3-methylpentyl)-	54965-05-8	0.74	0.09
14	2-Heptanone, 6-methyl	928-68-7	0.59	0.08
30	Cyclohexane, 1-ethyl-4-methyl-, cis-	4926-78-7	0.57	0.06
60	Tridecane, 4,8-dimethyl-	55030-62-1	0.57	0.09
6	Furan, tetrahydro-	109-99-9	0.55	0.07
62	Hexadecane	544-76-3	0.55	0.10
55	Dodecane, 3-methyl-	17312-57-1	0.54	0.06
12	3-Heptanone	106-35-4	0.54	0.05
3	1-Propanol	71-23-8	0.48	0.02
9	Cyclotrisiloxane, hexamethyl-	541-05-9	0.48	0.16
54	Tridecane, 2-methyl-	1560-96-9	0.48	0.04
34	Dodecane, 3-methyl-	17312-57-1	0.46	0.05
27	Undecane, 2-methyl-	7045-71-8	0.41	0.05
25	Undecane, 6-methyl-	17302-33-9	0.36	0.05
58	3-Dodecanone	1534-27-6	0.31	0.05

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
43	Cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.31	0.02
63	6-Tridecanone	22026-12-6	0.31	0.07
28	Decane, 3,8-dimethyl-	17312-55-9	0.30	0.04
46	2(3H)-Benzofuranone, 3a, 4,5,6- tetrahydro-trimethyl-	16778-26-0	0.30	0.03
47	3-Undecanone	2216-87-7	0.30	0.11
4	2-Butanone	78-93-3	0.26	0.01
48	Tridecane, 7-methyl-	26730-14-3	0.26	0.02
32	4-Undecene, 6-methyl-		0.24	0.01
50	C3-Decahydronaphthalene		0.24	0.03
17	1-Hexanol, 2-ethyl-	104-76-7	0.23	0.04
7	1H-Pyrazole, 3-methyl-	1453-58-3	0.23	0.05
26	Undecane, 4-methyl-	2980-69-0	0.21	0.02
16	Cyclotetrasiloxane, octamethyl-	556-67-2	0.21	0.20
2	Ethanol and butane, 2-methyl-		0.20	0.18
29	Decane, 2,4,6-trimethyl-	62108-27-4	0.20	0.02
20	1-Octanol	111-87-5	0.17	0.02
22	Octane, 6-ethyl-2-methyl-	62016-19-7	0.17	0.02
10	Nitric acid, butyl ester	928-45-0	0.17	0.01
11	1-Hexanol	111-27-3	0.17	0.03
64	3-Tridecanone	1534-26-5	0.17	0.06
65	Pentadecane	629-62-9	0.16	0.02
36	Cyclododecane	294-62-2	0.16	0.01
18	Oxirane, 2-ethyl-3-propyl-, cis-	56052-94-9	0.16	0.02
35	Decane, 2,3,7-trimethyl-	62238-13-5	0.16	0.02
45	Cyclohexane, 1,1,3,5-tetramethyl-	50876-32-9	0.15	0.27
19	2-Heptanone, 6-methyl-	928-68-7	0.15	0.02
23	Cyclohexane, pentyl-	4292-92-6	0.13	0.11
57	1,1'-Bicyclohexyl, 2-methyl-, cis-	50991-08-7	0.12	0.02

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
66	Benzenesulfonamide, N-butyl-	3622-84-2	0.097	0.088
38	4-Nonene, 5-butyl-	7367-38-6	0.085	0.074
5	Nitrous acid, butyl ester	544-16-1	0.062	0.110
8	1-Pentanol	71-41-0	0.062	0.110
52	Dodecane, 2,5-dimethyl-	56292-65-0	0.061	0.100
15	1-Heptanol	111-70-6	0.052	0.090
13	Nitric acid, pentyl ester	1002-16-0	0.049	0.085
51	Cyclohexane,1,3,5-trimethyl-2-octadecyl-	55282-34-3	0.048	0.084
21	2-Nonanone	821-55-6	0.046	0.080
31	Naphthalene, decahydro-2, 6-dimethyl-	1618-22-0	0.039	0.068
37	Naphthalene, decahydro-2, 3-dimethyl-	1008-80-6	0.039	0.068
24	Naphthalene, decahydro-2-methyl-	2958-76-1	0.037	0.064
Sum of tentatively identified compounds:			33.63	

1 CAS = Chemical Abstract Service.

2 Average of 3, 200 ml TST samples by ORNL, values listed are estimates.

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