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Accession #: D196058241

Document #: SD-WM-ER-426

Title/Desc:

TANK 241C112 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
6/1994 & 8/1994

ENGINEERING CHANGE NOTICE

Page 1 of 2

1. ECN 626286

Proj.
ECN

2. ECN Category (mark one) Supplemental ☐ Direct Revision ☒ Change ECN ☐ Temporary ☐ Standby ☐ Supersedure ☐ Cancel/Void ☐	3. Originator's Name, Organization, MSIN, and Telephone No. D. R. BRATZEL, 75640, S7-21, 373-3579	3a. USQ Required? ☐ Yes ☒ No	4. Date 09/27/95
	5. Project Title/No./Work Order No. TANK 241-C-112 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN JUNE 1994 AND AUGUST 1994	6. Bldg./Sys./Fac. No. 2704HV/200E	7. Approval Designator N/A
11a. Modification Work ☐ Yes (fill out Blk. 11b) ☒ No (NA Blks. 11b, 11c, 11d)	11b. Work Package No. N/A	11c. Modification Work Complete N/A Cog. Engineer Signature & Date	11d. Restored to Original Condition (Temp. or Standby ECN only) N/A Cog. Engineer Signature & Date
12. Description of Change Title change and complete rewrite.			
13a. Justification (mark one) Criteria Change ☒ Design Improvement ☐ Environmental ☐ Facility Deactivation ☐ As-Found ☐ Facilitate Const ☐ Const. Error/Omission ☐ Design Error/Omission ☐			
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 27 1995 <i>Stewart</i>

ENGINEERING CHANGE NOTICE				Page 2 of 2		1. ECN (use no. from pg. 1) 626286	
15. Design Verification Required		16. Cost Impact				17. Schedule Impact (days)	
		ENGINEERING		CONSTRUCTION			
☐ Yes		Additional ☐ \$		Additional ☐ \$		Improvement ☐	
☒ No		Savings ☐ \$		Savings ☐ \$		Delay ☐	

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SEP 27 1995

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Document Number: WHC-SD-WM-ER-426, REV 2

Document Title: Tank 241-C-112 Headspace Gas and Vapor
Characterization Results for Samples Collected in
June 1994 and August 1994

Release Date: 9/26/95

**This document was reviewed following the
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WHC Information Release Administration Specialist:

Kara Broz

9/26/95

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SUPPORTING DOCUMENT

1. Total Pages **39**

2. Title

TANK 241-C-112 HEADSPACE GAS AND VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
JUNE 1994 AND AUGUST 1994

3. Number

WHC-SD-WM-ER-426

4. Rev No.

2

5. Key Words

CHARACTERIZATION OBJECTIVES, TANK HEADSPACE,
SAMPLING EVENT, INORGANIC GASES, ORGANIC VAPORS

6. Author

Name: D. R. BRATZEL

Signature DR Bratzel 9/25/95

Organization/Charge Code 75640/N4AB1

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-C-112 Headspace Gas and Vapor Characterization Results for Samples Collected in June 1994 and August 1994

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Date Published
September 1995

Prepared for the U.S. Department of Energy
Office of Environmental Restoration and
Waste Management

Westinghouse
Hanford Company

P.O. Box 1970
Richland, Washington

Management and Operations Contractor for the
U.S. Department of Energy under Contract DE-AC06-87RL10930

Approved for Public Release

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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

Acknowledgements

The author wishes to thank Chris Simonen for her work verifying data and generating tables, and Shas Mattigod for his help with the construction and reviews of this document.

**Tank 241-C-112 Headspace Gas and Vapor Characterization Results
for Samples Collected in June 1994 and August 1994**

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank C-112 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 June 1994 sampling event. The tank C-112 headspace was sampled in June 1994 in accordance with *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991), 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 was collected to help in the evaluation of 1) headspace flammability, and 2) identification and quantification of compounds of toxicological concern.

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). However, current governing operating specifications for Watchlist tanks, such as tank C-112, 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-112 was vapor sampled in June 1994 using the *in situ* sampling (ISS) method, and again in August 1994 using the more robust vapor sampling system (VSS) method. Because the ISS sample volume flow measurement used during the June 1994 event was inherently less accurate than that of the VSS, the sorbent trap samples from the ISS event are not considered to be equivalent to those from the VSS sampling event (Huckaby et al. 1995). Furthermore, there are other discrepancies between results from the ISS and VSS methods that are not understood (Huckaby 1994a), and until the ISS method has been validated and the discrepancies resolved, results from early ISS events should be considered suspect.

Nevertheless, a brief description of the ISS event and hydrogen cyanide sampling results from the June 1994 ISS event are presented below, because this analyte was not sampled for during the VSS event. Huckaby et al. (1995) describe the bases for using the ISS method for hydrogen cyanide, and why it was not sampled for during the VSS event. All other results presented here are from the August 1994 VSS sampling event. Pingel (1994) provides sampling information for the June 1994 ISS event, and McVeety et al. (1995) describe sample preparation and analyses, and report results.

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 C-112 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 C-112 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank C-112 is the last tank in a 3-tank cascade with tanks C-110 and C-111, and is connected to tank C-111 (the second tank in the series) via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade line. Tank C-111 is also connected with tank C-110 (the first tank in the series) by a similar cascade line. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank C-110 or tank C-111 may be transferred to tank C-112 (unless the cascade lines are obstructed). However, as discussed in Section 3.5 below, headspace data from tank C-111 indicate that the inter-tank exchange of gases and vapors has little effect on the headspace composition of tank C-112.

The cascade of tanks C-110, C-111, and C-112 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 EVENTS

2.1 June 1994 *In Situ* Sampling Event

Tank C-112 was sampled using ISS methods on June 24, 1994 by WHC Sampling and Mobile Laboratories. This sampling was conducted to satisfy requirements of *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991). Samples for hydrogen cyanide were collected from a point approximately 7.9 m below the top of the flange on riser 4, between 2:00 p.m. and 3:25 p.m.

Huckaby et al. (1995) give a general description of the ISS method and equipment. Pingel (1994) provides field sampling information for the tank C-112 June 1994 ISS event, and Mahon (1995) provides revised sample volume measurements. In addition to the hydrogen cyanide results presented below, McVeety et al. (1995) 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-112 using the VSS on August 11, 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 28 °C. Air from the tank C-112 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 (SNL). 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 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 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 as given in Section 3.3. Inorganic analyte sorbent traps were prepared and analyzed by PNL, and SUMMATM canisters were prepared and analyzed by OGIST. Reports by Ligothke et al. (1995) and Rasmussen (1994) describe sample preparation and analyses.

Inorganic analyte sorbent trap analyses by PNL were completed within 14 days of sample collection (Ligothke 1995), which satisfied 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 3.

SUMMATM analyses by OGIST were initiated 8 days after samples were collected and apparently completed well within the WHC 60-day holding time requirement (Rasmussen 1994). OGIST SUMMATM data have been placed in square brackets both in Table 3-1 and elsewhere in this report to indicate they represent secondary results. Furthermore, OGIST was not operating under a WHC-approved quality assurance plan when samples were analyzed.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration in the headspace of tank C-112 is 22.7 ppmv. Ammonia concentrations higher than this level have been observed in the headspaces of other waste tanks. The relatively low ammonia concentration in tank C-112 may be related to the fact that only a small quantity of relatively cool waste is stored in tank C-112. Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 22.7 ppmv corresponds to less than 0.02 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

Hydrogen was measured to be an average [204 ppmv] in 3 SUMMATM canister samples by OGIST. In general, hydrogen is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, the [204 ppmv] hydrogen concentration in tank C-112 corresponds to less than 0.5 % of its LFL. At this level, hydrogen is not a flammability concern in tank C-112.

The average nitrous oxide concentration in the 3 OGIST SUMMATM samples was [544 ppmv]. Nitrous oxide has been detected in other passively ventilated waste tanks at average concentrations as high as 878 ppmv in tank U-103 (Ligothke et al. 1995b). 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-112 headspace.

3.2 Carbon Dioxide and Carbon Monoxide

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

The average measured headspace carbon dioxide concentration, [102 ppmv], is below the normal ambient air concentration of about 350 to 400 ppmv. Lower-than-ambient carbon dioxide concentrations are typical for the passively ventilated waste tanks. 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. It is reasonable to expect the level of carbon dioxide in a tank headspace will therefore depend on the tank's breathing rate, and the pH and surface area of aqueous waste (i.e., supernate, interstitial liquid, and condensate) in the tank.

Carbon monoxide in the tank C-112 headspace, at about [0.92 ppmv], is above its concentration 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 concentration 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.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank C-112 headspace were determined to be 0.62 ppmv and ≤ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank C-112. 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-112 headspace.

The water vapor concentration of tank C-112 was determined to be about 22.3 mg/L, at the tank headspace temperature of 28 °C and pressure of 989 mbar (742 torr), (WHC 1995). This corresponds to water vapor partial pressure of 31.0 mbar (23.2 torr), to a dew point of 24.6 °C, and to a relative humidity of 82 %. The water vapor content of the tank C-112 headspace is typical of other 241-C farm tanks.

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

3.4 Hydrogen Cyanide

Analysis of the hydrogen cyanide sorbent traps collected during the June 1994 ISS event indicated the concentration of this analyte to be below 0.01 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-112. No hydrogen cyanide has been detected in any of the 10 waste tank headspaces sampled for this analyte.

3.5 Discussion of Inorganic Gases and Vapors

Aside from water vapor and carbon dioxide, the most abundant waste constituents in the tank C-112 headspace are nitrous oxide, hydrogen, and ammonia. These have been detected in most tank

headspaces sampled to date, and are usually the dominant gas species. The concentrations of nitrous oxide and hydrogen are higher in tank C-112 than in most other waste tanks that have been sampled, but the ammonia concentration in tank C-112 is lower.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are good for the methods used at the concentrations reported. Relative standard deviations range from 1 % for the OGIST measurement of carbon dioxide, to about 8 % for the PNL measurement of nitric oxide. 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.

As discussed briefly in Section 1.4, it is possible that gases and vapors generated by the waste in tanks C-110 and C-111 could be transferred to tank C-112 via the cascade lines. Table 3-2 lists the concentrations of selected inorganic gases and vapors in tanks C-110, C-111, and C-112. If a significant exchange of gases and vapors were taking place between adjacent tanks, either their headspace compositions would be very similar, or all headspace waste constituents detected in one tank would be at an equal or higher concentration (and carbon dioxide would be at a lower concentration) in the other tank. Data in Table 3-2 are consistent with the premise that air, gases, and vapors from tank C-111 could be flowing into tank C-112, but do not constitute proof that this indeed is occurring.

4.0 ORGANIC VAPORS

Organic vapors in the tank C-112 headspace were sampled using SUMMA™ canisters, which were analyzed at PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. None of the positively or tentatively identified organic analytes were at or above levels of concern. Both laboratories used a gas chromatograph (GC) equipped with a mass spectrometer (MS) detector to separate, identify, and quantitate the analytes. A quantitative measurement of the TNMOC concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method was also performed by OGIST on SUMMA™ canister samples from the June 1994 ISS event. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1994), Ligothke et al. (1995a), and Rasmussen (1994).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank C-112. These results were produced at PNL quality assurance impact level 3. All PNL analyses were not completed until 121 days after sample collection, however, and did not satisfy the administratively chosen 60-day holding time (Keller 1994). No holding time study has been performed to determine the stability of organic 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. 1994). 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 from the 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 from tank C-103.

Table 4-1 lists the 2 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, Ligothke et al. 1995a). Except for about 0.0035 ppmv of toluene detected in 1 SUMMA™ canister sample, none of the 40 TO-14 analytes were observed to be above the 0.002 ppmv quantitation limit of the analyses. The results for methane are those of OGIST (Rasmussen 1994). Averages reported are from analyses of 3 SUMMA™ canister samples.

ORNL positively identified 22 of 27 target analytes selected by WHC (5 analytes were below detection limits). Despite calibration of the instrument over about a 20-fold concentration range, none of these analytes were within the calibration range in all 4 TST samples analyzed. Tables 4-2 and 4-3 list the analytes and their average concentrations from the analysis of 4 TST samples. Segregated in Table 4-3 is 1 analyte, 1-butanol, for which the ORNL practical holding time was exceeded. Data in Tables 4-2 and 4-3 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. Jenkins et al. (1995) describe the ORNL practical holding time study, and report the practical holding times of butanal and 1-butanol are 1 and 17 days, respectively. Because TST analyses were not completed until 33 days after sample collection (Jenkins 1995b), the results for these 2 compounds may have been affected. It is possible that butanal was not identified in the tank C-112 TST samples because the practical holding time for this compound was exceeded. It should also 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. These compounds are listed in Table 4-4 with the ORNL and PNL measured concentrations. ORNL detected trace amounts of dichloromethane and benzene, but these were both below the limit of detection of PNL (0.002 ppmv). The 0.0035 ppmv of toluene detected in a single PNL sample is not supported by the ORNL analyses.

The 2 most abundant analytes in Tables 4-1 through 4-3 are methane and ethanenitrile. At 1.013 ppmv, the methane concentration in tank C-112 is above ambient levels, which are typically about 0.2 ppmv. Elevated methane concentrations have been observed in other waste tank headspaces, and methane is probably formed during the chemical and radiolytic degradation of organic wastes. For methane, 1.0 ppmv corresponds to roughly 0.002 % of its LFL. Similarly, ethanenitrile, at 3.0 ppmv, presents virtually no flammability risk.

4.2 Tentatively Identified Organic Analytes

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

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and SUMMA™ samples. Analyses of the samples are designed to recover, separate, and identify the organic vapors in the samples. TSTs are not good for collecting highly volatile compounds (i.e., molecules more volatile than propane), but are quite good for most others. In contrast, the recovery of very low volatility compounds (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 tentatively identified compounds recovered from SUMMA™ samples, in the order by which the eluted chromatographically, are given in Table 4-5 with estimated concentrations. Only non-zero results are included in the reported averages. Estimated concentrations are in mg/m³, 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 4-6. Compounds are listed in Table 4-6 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table 4-6 are all 4-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. Because the list of tentatively identified organic compounds in TST samples is particularly long and locating any given compound may be difficult, the list has been sorted alphanumerically by compound name in Table 4-7. Table 4-8 gives the same list, sorted in order of decreasing estimated concentration. Numbers in the first columns of Tables 4-7 and 4-8 (Cmpd #) identify the location of the compound in Table 4-6. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Ligothke et al. (1995a), respectively, and should be reviewed before this data are used for decision making. Results in Tables 4-5 through 4-8 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 70 and 76 in Table 4-6). 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 4-5 and 4-6 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 [3.4 mg/m³], with a standard deviation of [0.1 mg/m³]. This is a relatively low TNMOC concentration compared to other passively ventilated tanks that have been sampled. For comparison, the TNMOC concentration in clean ambient air may range from 0.03 to 0.1 mg/m³, in polluted city air it may be 0.3 to 0.4 mg/m³, and tank C-103 has an estimated [2,000 to 5,000 mg/m³] (Rasmussen and Einfeld 1994).

4.4 Discussion of Organic Analytes

Some of the compounds listed in Tables 4-1 through 4-8 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 the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-dodecane, n-tridecane, n-tetradecane, n-pentadecane) that were used as a diluent for tributyl phosphate in several Hanford site processes.

Notably absent from the tank C-112 headspace are the semivolatile cyclic alkanes (e.g., methylated decahydronaphthalenes, cyclopentanes, and cyclohexanes) that have been observed in the 241-BY tank farm. This suggests that the semivolatile organic waste in tank C-112 is probably from a process or period when a relatively pure form of semivolatile NPHs was used as a process diluent.

Most of the compounds in Tables 4-1 through 4-8 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 is thought 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 4-8 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 alcohols are 1-alkanols, 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. These have generally not been observed to be as numerous in other NPH-rich tank headspaces, which tend to be dominated by aldehydes, ketones, alkanes, and alkenes.

5.0 SUMMARY

The tank C-112 headspace was sampled in June 1994 and again in August 1994 for gases and vapors to address flammability and industrial hygiene concerns. Collection and analysis of samples has been reported. It was determined that no headspace constituents exceeded the flammability or industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

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Table 2-1
Tank C-112 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device ¹	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	1.0	Organic vapors	8 tank air samples
		4.0	Organic vapors	8 tank air samples + 2 trip blanks + 2 field 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

¹ Sampling Temperature ~ 50 ° C

Table 3-1
**Tank C-112 Inorganic Gas and Vapor Concentrations --
 Analyses by Oregon Graduate Institute of Science and Technology and by Pacific Northwest Laboratory**

Compound	CAS ¹ Number	Sample Type	Number of samples	Average ² (ppmv)	Standard Deviation (ppmv)	RSD ^{2,3} (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	22.7	0.5	2
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	[102]	[1]	[1]
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	[0.92]	[0.02]	[3]
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	[204]	[5]	[3]
Hydrogen Cyanide ⁴ , HCN	74-90-8	Sorbent Trap	3	< 0.01	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.62	0.05	8
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	[544]	[9]	[2]
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	31,300 (22.3 mg/L)	1,800 (1.3 mg/L)	6

1 CAS = Chemical Abstracts Service.

2 Bracketed values are from OGI/ST 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 June 1994 ISS event.

Table 3-2
Comparison of Tank C-110, C-111, and C-112 Headspace Constituents --
Inorganic Analyses by Oregon Graduate Institute of Science and Technology,
and Organic Analyses by Oak ridge National Laboratory¹

Tank:	C-110 ²	C-111 ³	C-112
Date sampled, (mo/day/yr)	8/8/94	9/13/94	8/11/94
Headspace temperature, (°C)	21.9	27	28
Sampling Temperature, (°C)	50	50	50
Ammonia, (ppmv)	124	5.6	22.7
Hydrogen, (ppmv)	[12]	[12.4]	[204]
Carbon dioxide, (ppmv)	[42]	[198]	[102]
Carbon monoxide, (ppmv)	[0.7]	[0.10] ⁴	[0.92]
Nitric oxide, (ppmv)	0.08	0.62	0.62
Nitrogen dioxide, (ppmv)	≤ 0.06	≤ 0.08	≤ 0.02
Nitrous oxide, (ppmv)	[9.4]	[99.3]	[544]
Water vapor, (mg/m ³)	12.4	22.2	22.3
Water vapor, (% relative humidity)	64	86	82
Ethanenitrile (acetonitrile), (ppmv)	(0.17)	0.0093	(3.0)
Propanone (acetone), (ppmv)	(0.21)	0.0080	(0.078)
1-Butanol, (ppmv)	(0.73)	(0.0016)	0.0044
n-Dodecane, (ppmv)	(0.084)	(0.00054)	(0.00043)
n-Tridecane, (ppmv)	(0.15)	(0.0012)	(0.00060)
Total nonmethane organic compounds by EPA TO-12 method, (mg/m ³)	[22.2]	[0.18]	[3.4]

1 Where PNL inorganic gas or vapor data was unavailable for tanks C-111 and C-112, 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 and Bratzel 1995a.

3 Data are from Huckaby and Bratzel 1995b.

4 Carbon monoxide for tank C-111 is from the August 1993 ISS event (Huckaby and Bratzel 1995b).

Table 4-1
Tank C-112 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	[1.013]	[0.006]	[0.6]
2	Toluene ⁵	108-88-3	0.0035	--	--

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 Detected in only 1 sample.

Table 4-2
Tank C-112 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	3.0	0.9	31
2	Propanone (acetone)	67-64-1	0.078	0.018	23
3	Dichloromethane (methylene chloride)	75-09-2	0.00018	--	--
4	Propanenitrile	107-12-0	0.023	0.006	26
5	n-Hexane	110-54-3	0.00009	0.00001	13
6	Benzene	71-43-2	0.00011	0.00002	22
7	n-Butanenitrile	109-74-0	0.0032	0.0007	23
8	2-Pentanone	107-87-9	0.0012	0.0005	43
9	n-Heptane	142-82-5	0.00071	0.00054	77
10	Toluene	108-88-3	<0.0003	--	--
11	n-Pentanenitrile	110-59-8	0.00037	0.00006	15
12	2-Hexanone	591-78-6	0.00031	0.00008	27
13	n-Octane	111-65-9	0.00016	0.00007	46
14	n-Hexanenitrile	628-73-9	0.00017	0.00002	9
15	2-Heptanone	110-43-0	0.00021	0.00005	22
16	n-Nonane	111-84-2	0.00012	0.00005	45
17	n-Heptanenitrile	629-08-3	0.00015	0.00002	14
18	2-Octanone	111-13-7	0.00010	0.00001	11
19	n-Octanenitrile	124-12-9	0.000063	0.000014	21
20	n-Nonanenitrile	2243-27-8	0.000087	0.000013	15
21	n-Dodecane	112-40-3	0.00043	0.00008	19
22	n-Tridecane	629-50-5	0.00060	0.00007	11

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 4 TST samples: 3 were 4-L and 1 was 1-L.

4 RSD = Relative Standard Deviation. Burnum (1995) specifies the RSD should be less than 25 %.

Table 4-3

**Tank C-112 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	0.0044	0.0017	39

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

2 CAS = Chemical Abstract Service.

3 Average of 4 TST samples: 3 were 4-L and 1 was 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 4-4
Tank C-112 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 (%)
Dichloromethane (methylene chloride)	75-09-2	0.00018	< 0.002	--
Benzene	71-43-2	0.00011	< 0.002	--
Toluene	108-88-3	<0.0003	0.0035	> 168

1 CAS = Chemical Abstract Service.

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

3 Average of 3 sample analyses.

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

Table 4-5
Tank C-112 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviations (mg/m ³)
1	Ethanal (acetaldehyde)	75-07-0	0.17	0.09
2	Ethanenitrile (acetonitrile)	75-05-8	1.99	0.09
3	Propanone (acetone)	67-64-1	0.56	0.01
4	Methyl Nitrate	598-58-3	0.20	0.01
5	Propanenitrile	107-12-0	0.07	0.05
Sum of tentatively identified compounds:			2.99	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples, values listed are estimates.

Table 4-6
Tank C-112 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	Trichlorofluoromethane	75-69-4	0.001	0.002
2	Nitric acid, methyl ester	598-58-3	0.030	0.009
3	Nitric acid, ethyl ester	625-58-1	0.003	0.003
4	Propanenitrile, 2,2-dimethyl-	630-18-2	0.002	0.003
5	Acetic acid	64-19-7	0.003	0.003
6	2-Butanone, 3,3-dimethyl-	75-97-8	0.001	0.001
7	Siloxane and others		0.001	0.001
8	Nitric acid, propyl ester	627-13-4	0.002	0.002
9	Cyclopropanecarbonitrile	5500-21-0	0.006	0.005
10	Propane, 2-methyl-2-nitro-	594-70-7	0.010	0.007
11	Alkanol		0.001	0.002
12	Nitric acid, ester		0.001	0.001
13	Siloxane and others		0.006	0.005
14	Hexanal	66-25-1	0.001	0.002
15	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-, trans-	24405-16-1	0.005	0.011
16	1-Propanol, 2,2-dimethyl, nitrate	926-42-1	0.001	0.001
17	Cyclotrisiloxane, hexamethyl-	541-05-9	0.009	0.009
18	Heptanal	111-71-7	0.001	0.001
19	2-Heptanone, 3-methyl-	2371-19-9	0.002	0.002
20	Oxirane, ethenyl-	930-22-3	0.018	0.005
21	2-Heptanone, 6-methyl-	928-68-7	0.001	0.001
22	Cyclotetrasiloxane, octamethyl-	556-67-2	0.005	0.003
23	2-Heptanone, 4-methyl and others	110-43-0	0.002	0.001
24	Octanal	124-13-0	0.001	0.002
25	2H-Pyran-2-one, tetrahydro-6,6-dimethyl-	2610-95-9	0.002	0.001
26	1-Hexanol,2-ethyl-	104-76-7	0.0005	0.001

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	Isothiazole	288-16-4	0.001	0.001
28	Ethanone, 1-phenyl-	98-86-2	0.004	0.003
29	Benzenemethanol, a,a,-dimethyl-	617-94-7	0.001	0.001
30	Nonanal	124-19-6	0.004	0.002
31	1-Decene and others		0.001	0.001
32	Decanal	112-31-2	0.003	0.002
33	Undecane, 3,6-dimethyl-	17301-28-9	0.001	0.001
34	Decane, 2,2,6-trimethyl-	62237-97-2	0.001	0.001
35	C13-Alkane		0.001	0.001
36	Alkane		0.0003	0.001
37	1-Hexanol, 2-ethyl-	104-76-7	0.0004	0.001
38	1H-Azepin-1-amine,N-ethylidenehexahydro-	75268-01-8	0.008	0.002
39	Alkane and others		0.001	0.003
40	Heptane, 2,2,4,6,6-pentamethyl-	13475-82-6	0.006	0.001
41	C13-Alkane		0.002	0.001
42	Nonane, 3-methyl-5-propyl-	31081-18-2	0.002	0.002
43	C13-Alkane		0.002	0.001
44	C13-Alkane		0.001	0.001
45	Mixture		0.0003	0.001
46	Decane, 2,6,8-trimethyl-	62108-26-3	0.001	0.001
47	Alkane		0.0003	0.001
48	Undecane, 3,5-dimethyl-	17312-81-1	0.0003	0.001
49	Alkane		0.0003	0.001
50	C13-Alkane		0.002	0.001
51	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	74367-34-3	0.0004	0.001
52	C6 ester of butanoic acid		0.0004	0.001
53	Tetradecane	629-59-4	0.005	0.000
54	C15-Alkane		0.002	0.001

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	1-Hexadecanol	29354-98-1	0.0003	0.001
56	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	0.0003	0.001
57	Pentadecane	629-62-9	0.002	0.001
58	Dodecanoic acid	143-07-7	0.004	0.002
59	C16-alkane		0.0005	0.001
60	Heptadecane	629-78-7	0.0004	0.001
61	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	0.037	0.014
62	Alkane		0.002	0.005
63	Benzenamine, N-phenyl-	122-39-4	0.005	0.003
64	Alkane		0.001	0.002
65	Benzenesulfonamide, N-alkyl		0.001	0.002
66	Phenoxy Benzaldehyde		0.001	0.001
67	Nonadecane	629-92-5	0.0004	0.001
68	1-Hexadecanol	36653-82-4	0.0003	0.001
69	1,1'-Biphenyl,2,2'-diethyl-	13049-35-9	0.001	0.001
70	Tetradecanoic acid	544-63-8	0.020	0.008
71	Alkanoic acid and others		0.001	0.003
72	Alkanoic acid and others		0.001	0.003
73	Hexanedioic acid, dioctyl ester	123-79-5	0.004	0.008
74	Benzenesulfonamide, N-butyl-	3622-84-2	0.081	0.042
75	Alkane		0.000	0.001
76	Tetradecanoic acid	544-63-8	0.024	0.036
77	2-Octadecenal	56554-96-2	0.0003	0.001
78	Alkane		0.002	0.002
79	9-Hexadecenoic acid	2091-29-4	0.006	0.007
80	Cyclohexanecarboxylic acid, 2-(1,1-dimethylethyl)-, trans-	27392-16-1	0.001	0.001

WHC-SD-WM-ER-426 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
81	Alkene		0.005	0.007
82	Hexadecanoic acid	57-10-3	0.035	0.013
83	Phthalate		0.001	0.001
84	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.001	0.001
85	Alkane		0.001	0.001
86	10-demethylsqualene		0.003	0.006
Sum of tentatively identified compounds:			0.41	

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples: 3 were 4-L and 1 was 1-L, values listed are estimates.

Table 4-7
Tank C-112 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)
55	1-Hexadecanol	29354-98-1	0.0003	0.001
26	1-Hexanol,2-ethyl-	104-76-7	0.0005	0.001
31	1-Decene and others		0.001	0.001
16	1-Propanol, 2,2-dimethyl, nitrate	926-42-1	0.001	0.001
68	1-Hexadecanol	36653-82-4	0.0003	0.001
37	1-Hexanol, 2-ethyl-	104-76-7	0.0004	0.001
38	1H-Azepin-1-amine,N-ethylidenehexahydro-	75268-01-8	0.008	0.002
6	2-Butanone, 3,3-dimethyl-	75-97-8	0.001	0.001
23	2-Heptanone, 4-methyl and others	110-43-0	0.002	0.001
21	2-Heptanone, 6-methyl-	928-68-7	0.001	0.001
77	2-Octadecenal	56554-96-2	0.0003	0.001
19	2-Heptanone, 3-methyl-	2371-19-9	0.002	0.002
15	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-, trans-	24405-16-1	0.005	0.011
25	2H-Pyran-2-one, tetrahydro-6,6-dimethyl-	2610-95-9	0.002	0.001
52	C6 ester of butanoic acid		0.0004	0.001
79	9-Hexadecenoic acid	2091-29-4	0.006	0.007
86	10-demethylsqualene		0.003	0.006
69	1,1'-Biphenyl,2,2'-diethyl-	13049-35-9	0.001	0.001
41	C13-Alkane		0.002	0.001
50	C13-Alkane		0.002	0.001
35	C13-Alkane		0.001	0.001
44	C13-Alkane		0.001	0.001
43	C13-Alkane		0.002	0.001
54	C15-Alkane		0.002	0.001
59	C16-alkane		0.0005	0.001

WCH-SD-WM-ER-426 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
56	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	0.0003	0.001
5	Acetic acid	64-19-7	0.003	0.003
62	Alkane		0.002	0.005
36	Alkane		0.0003	0.001
64	Alkane		0.001	0.002
39	Alkane and others		0.001	0.003
85	Alkane		0.001	0.001
49	Alkane		0.0003	0.001
78	Alkane		0.002	0.002
75	Alkane		0.000	0.001
47	Alkane		0.0003	0.001
72	Alkanoic acid and others		0.001	0.003
71	Alkanoic acid and others		0.001	0.003
11	Alkanol		0.001	0.002
81	Alkene		0.005	0.007
63	Benzenamine, N-phenyl-	122-39-4	0.005	0.003
29	Benzenemethanol, a,a,-dimethyl-	617-94-7	0.001	0.001
74	Benzenesulfonamide, N-butyl-	3622-84-2	0.081	0.042
65	Benzenesulfonamide, N-alkyl		0.001	0.002
80	Cyclohexanecarboxylic acid, 2-(1,1-dimethylethyl)-, trans-	27392-16-1	0.001	0.001
9	Cyclopropanecarbonitrile	5500-21-0	0.006	0.005
22	Cyclotetrasiloxane, octamethyl-	556-67-2	0.005	0.003
17	Cyclotrisiloxane, hexamethyl-	541-05-9	0.009	0.009
32	Decanal	112-31-2	0.003	0.002
46	Decane, 2,6,8-trimethyl-	62108-26-3	0.001	0.001
34	Decane, 2,2,6-trimethyl-	62237-97-2	0.001	0.001
58	Dodecanoic acid	143-07-7	0.004	0.002

WHC-SD-WM-ER-426 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
28	Ethanone, 1-phenyl-	98-86-2	0.004	0.003
60	Heptadecane	629-78-7	0.0004	0.001
18	Heptanal	111-71-7	0.001	0.001
40	Heptane, 2,2,4,6,6-pentamethyl-	13475-82-6	0.006	0.001
82	Hexadecanoic acid	57-10-3	0.035	0.013
84	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.001	0.001
14	Hexanal	66-25-1	0.001	0.002
73	Hexanedioic acid, dioctyl ester	123-79-5	0.004	0.008
27	Isothiazole	288-16-4	0.001	0.001
45	Mixture		0.0003	0.001
8	Nitric acid, propyl ester	627-13-4	0.002	0.002
12	Nitric acid, ester		0.001	0.001
3	Nitric acid, ethyl ester	625-58-1	0.003	0.003
2	Nitric acid, methyl ester	598-58-3	0.030	0.009
67	Nonadecane	629-92-5	0.0004	0.001
30	Nonanal	124-19-6	0.004	0.002
42	Nonane, 3-methyl-5-propyl-	31081-18-2	0.002	0.002
24	Octanal	124-13-0	0.001	0.002
20	Oxirane, ethenyl-	930-22-3	0.018	0.005
57	Pentadecane	629-62-9	0.002	0.001
66	Phenoxy Benzaldehyde		0.001	0.001
83	Phthalate		0.001	0.001
10	Propane, 2-methyl-2-nitro-	594-70-7	0.010	0.007
4	Propanenitrile, 2,2-dimethyl-	630-18-2	0.002	0.003
51	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	74367-34-3	0.0004	0.001
61	Propanoic acid, 2-methyl-,1-(1,1-dimethylethyl)-2-methyl-1,3- propanediyl ester	74381-40-1	0.037	0.014

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
7	Siloxane and others		0.001	0.001
13	Siloxane and others		0.006	0.005
53	Tetradecane	629-59-4	0.005	0.000
76	Tetradecanoic acid	544-63-8	0.024	0.036
70	Tetradecanoic acid	544-63-8	0.020	0.008
1	Trichlorofluoromethane	75-69-4	0.001	0.002
48	Undecane, 3,5-dimethyl-	17312-81-1	0.0003	0.001
33	Undecane, 3,6-dimethyl-	17301-28-9	0.001	0.001
Sum of tentatively identified compounds:			0.41	

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples: 3 were 4-L and 1 was 1-L, values listed are estimates.

Table 4-8
Tank C-112 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)
74	Benzenesulfonamide, N-butyl-	3622-84-2	0.081	0.042
61	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	0.037	0.014
82	Hexadecanoic acid	57-10-3	0.035	0.013
2	Nitric acid, methyl ester	598-58-3	0.030	0.009
76	Tetradecanoic acid	544-63-8	0.024	0.036
70	Tetradecanoic acid	544-63-8	0.020	0.008
20	Oxirane, ethenyl	930-22-3	0.018	0.005
10	Propane, 2-methyl-2-nitro-	594-70-7	0.010	0.007
17	Cyclotrisiloxane, hexamethyl-	541-05-9	0.009	0.009
38	1H-Azepin-1-amine, N-ethylidenehexahydro-	75268-01-8	0.008	0.002
9	Cyclopropanecarbonitrile	5500-21-0	0.006	0.005
40	Heptane, 2,2,4,6,6-pentamethyl-	13475-82-6	0.006	0.001
13	Siloxane and others		0.006	0.005
79	9-Hexadecenoic acid	2091-29-4	0.006	0.007
15	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-, trans-	24405-16-1	0.005	0.011
53	Tetradecane	629-59-4	0.005	0.000
63	Benzenamine, N-phenyl-	122-39-4	0.005	0.003
22	Cyclotetrasiloxane, octamethyl-	556-67-2	0.005	0.003
81	Alkene		0.005	0.007
58	Dodecanoic acid	143-07-7	0.004	0.002
73	Hexanedioic acid, dioctyl ester	123-79-5	0.004	0.008
28	Ethanone, 1-phenyl-	98-86-2	0.004	0.003
30	Nonanal	124-19-6	0.004	0.002
5	Acetic acid	64-19-7	0.003	0.003

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
3	Nitric acid, ethyl ester	625-58-1	0.003	0.003
86	10-demethylsqualene		0.003	0.006
32	Decanal	112-31-2	0.003	0.002
25	2H-Pyran-2-one, tetrahydro-6,6-dimethyl-	2610-95-9	0.002	0.001
4	Propanenitrile, 2,2-dimethyl-	630-18-2	0.002	0.003
57	Pentadecane	629-62-9	0.002	0.001
62	Alkane		0.002	0.005
54	C15-Alkane		0.002	0.001
8	Nitric acid, propyl ester	627-13-4	0.002	0.002
50	C13-Alkane		0.002	0.001
78	Alkane		0.002	0.002
23	2-Heptanone, 4-methyl and others	110-43-0	0.002	0.001
43	C13-Alkane		0.002	0.001
19	2-Heptanone, 3-methyl-	2371-19-9	0.002	0.002
42	Nonane, 3-methyl-5-propyl-	31081-18-2	0.002	0.002
41	C13-Alkane		0.002	0.001
18	Heptanal	111-71-7	0.001	0.001
39	Alkane and others		0.001	0.003
21	2-Heptanone, 6-methyl-	928-68-7	0.001	0.001
44	C13-Alkane		0.001	0.001
16	1-Propanol, 2,2-dimethyl, nitrate	926-42-1	0.001	0.001
46	Decane, 2,6,8-trimethyl-	62108-26-3	0.001	0.001
35	C13-Alkane		0.001	0.001
14	Hexanal	66-25-1	0.001	0.002
12	Nitric acid, ester		0.001	0.001
34	Decane, 2,2,6-trimethyl-	62237-97-2	0.001	0.001
11	Alkanol		0.001	0.002
33	Undecane, 3,6-dimethyl-	17301-28-9	0.001	0.001

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
7	Siloxane and others		0.001	0.001
29	Benzenemethanol, a,a,-dimethyl-	617-94-7	0.001	0.001
6	2-Butanone, 3,3-dimethyl-	75-97-8	0.001	0.001
31	1-Decene and others		0.001	0.001
24	Octanal	124-13-0	0.001	0.002
27	Isothiazole	288-16-4	0.001	0.001
1	Trichlorofluoromethane	75-69-4	0.001	0.002
80	Cyclohexanecarboxylic acid, 2-(1,1-dimethylethyl)-, trans-	27392-16-1	0.001	0.001
71	Alkanoic acid and others		0.001	0.003
72	Alkanoic acid and others		0.001	0.003
85	Alkane		0.001	0.001
64	Alkane		0.001	0.002
65	Benzenesulfonamide, N-alkyl		0.001	0.002
66	Phenoxy Benzaldehyde		0.001	0.001
83	Phthalate		0.001	0.001
84	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.001	0.001
69	1,1'-Biphenyl,2,2'-diethyl-	13049-35-9	0.001	0.001
26	1-Hexanol,2-ethyl-	104-76-7	0.0005	0.001
59	C16-alkane		0.0005	0.001
52	C6 ester of butanoic acid		0.0004	0.001
51	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	74367-34-3	0.0004	0.001
67	Nonadecane	629-92-5	0.0004	0.001
60	Heptadecane	629-78-7	0.0004	0.001
37	1-Hexanol, 2-ethyl-	104-76-7	0.0004	0.001
77	2-Octadecenal	56554-96-2	0.0003	0.001
47	Alkane		0.0003	0.001
45	Mixture		0.0003	0.001

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
48	Undecane, 3,5-dimethyl-	17312-81-1	0.0003	0.001
56	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	0.0003	0.001
36	Alkane		0.0003	0.001
49	Alkane		0.0003	0.001
68	1-Hexadecanol	36653-82-4	0.0003	0.001
55	1-Hexadecanol	29354-98-1	0.0003	0.001
75	Alkane		0.000	0.001
Sum of tentatively identified compounds:			0.41	

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples: 3 were 4-L and 1 was 1-L, values listed are estimates.