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Accession #: D196054975

Document #: SD-WM-ER-510

Title/Desc:

TANK 241U103 HEADSPACE GAS & VAPOR
CHARACTERIZATION REASULTS FOR SAMPLES COLLECTED
IN 2/1995

Sta 4
SEP 27 1995

ENGINEERING DATA TRANSMITTAL

Page 1 of 1
1. EDT No 613581

2. To: (Receiving Organization) DISTRIBUTION		3. From: (Originating Organization) TWRS/CHARACTERIZATION PROJECT		4. Related EDT No.: N/A					
5. Proj./Prog./Dept./Div.: TWRS/CHAR PROJECT		6. Cog. Engr.: D. R. BRATZEL		7. Purchase Order No.: N/A					
8. Originator Remarks: N/A				9. Equip./Component No.: N/A					
				10. System/Bldg./Facility: 2704HV/200E					
11. Receiver Remarks:				12. Major Assm. Dwg. No.: N/A					
				13. Permit/Permit Application No.: N/A					
				14. Required Response Date: 09/27/95					
15. DATA TRANSMITTED									
(A) Item No.	(B) Document/Drawing No.	(C) Sheet No.	(D) Rev. No.	(E) Title or Description of Data Transmitted	(F) Approval Designator	(G) Reason for Transmittal	(H) Originator Disposition	(I) Receiver Disposition	
1	WHC-SD-WM-ER-510		0	TANK 241-U-103 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN FEBRUARY 1995	N/A TJD 9/27/95	1	1		
16. KEY									
Approval Designator (F)		Reason for Transmittal (G)			Disposition (H) & (I)				
E, S, Q, D or N/A (see WHC-CM-3-5, Sec.12.7)		1. Approval 2. Release 3. Information 4. Review 5. Post-Review 6. Dist. (Receipt Acknow. Required)			1. Approved 2. Approved w/comment 3. Disapproved w/comment 4. Reviewed no/comment 5. Reviewed w/comment 6. Receipt acknowledged				
17. SIGNATURE/DISTRIBUTION (See Approval Designator for required signatures)									
(G) Reason	(H) Disp.	(J) Name	(K) Signature	(L) Date	(M) MSIN	(J) Name	(K) Signature	(L) Date	(M) MSIN
1	1	Cog. Eng. D. R. BRATZEL		9/27/95					
1	1	Cog. Mgr. T. J. KELLEY		9/27/95					
		QA							
		Safety							
		Env.							
18. D. R. BRATZEL Signature of EDT Originator 9/27/95 Date									
19. N/A Authorized Representative Date for Receiving Organization									
20. T. J. KELLEY Cogizant Manager 9/27/95 Date									
21. DOE APPROVAL (if required) Ctrl. No. ☐ Approved ☐ Approved w/comments ☐ Disapproved w/comments									

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RELEASE AUTHORIZATION

Document Number: WHC-SD-WM-ER-510, REV 0

Document Title: Tank 241-U-103 Headspace Gas and Vapor
Characterization Results for Samples Collected in
February 1995

Release Date: 9/27/95

**This document was reviewed following the
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SUPPORTING DOCUMENT

1. Total Pages 34

2. Title

TANK 241-U-103 HEADSPACE GAS AND VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
FEBRUARY 1995

3. Number

WHC-SD-WM-ER-510

4. Rev No.

0

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.

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Tank 241-U-103 Headspace Gas and Vapor Characterization Results for Samples Collected in February 1995

J. L. Huckaby
Pacific Northwest Laboratories

D. R. Bratzel
Westinghouse Hanford Company

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
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%
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
wt%	percent by weight

Acknowledgements

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

Tank 241-U-103 Headspace Gas and Vapor Characterization Results
for Samples Collected in February 1995

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank U-103 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 U-103 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 1994). However, current governing operating specifications for single shell waste tanks, such as tank U-103 specify that combustible constituents be maintained at or below 20 % of the LFL (WHC 1995b).

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 headspace characterization data presented here are from a single sampling event. Samples collected are thought to have been representative of the tank U-103 headspace when the tank was sampled, and sample analyses were designed to provide a reasonably accurate and complete

characterization of the significant headspace constituents (Meacham et al. 1995). No assessment has been made of how the tank U-103 headspace composition changes with time, though studies of tank C-103 suggest that composition changes probably occur very slowly in the passively ventilated tanks (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank U-103 is the third tank in a 3-tank cascade with tanks U-101 and U-102. It is connected to tank U-102 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade line. A similar line connects tanks U-101 and U-102. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank U-101 or tank U-102 may be transferred to tank U-103 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data are available for tank U-102 to assess their potential transfer of gases and vapors to tank U-103.

The cascade of tanks U-101, U-102, and U-103 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 U-103 using the vapor sampling system (VSS) on February 15, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-U-103 Tank Characterization Plan* (Carpenter 1995). The tank headspace temperature was determined to be 29 °C. Air from the U-103 headspace was withdrawn from a single elevation via a 6.1-m long heated sampling probe mounted in riser 9, 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 11:03 a.m. and 2:34 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 et al (1995). The sampling equipment, sample collection sequence, sorbent trap sample air flow rates and flow times, chain of custody information, and a discussion of the sampling event itself are given in WHC (1995b).

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,1} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions and are given in Section 3.3. All inorganic gas and vapor tank samples, ambient air samples, and trip and field blanks were prepared and analyzed by PNL per PNL quality assurance impact level 2 procedures (Ligotke et al. 1995).

PNL analyses of SUMMATM canisters and sorbent traps for permanent gases and inorganic compounds were performed 30 and 22 days, respectively, after sample collection (Ligotke 1995). Thus these analyses satisfied the 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994). It should be noted that these inorganic compounds (i.e., the permanent gases) would be expected to be very stable in the SUMMATM canisters, and the results may not have been affected even if the 60-day holding time requirements had been exceeded.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration from 6 ammonia sorbent trap samples is 730 ppmv. This is relatively high compared to the other passively ventilated tanks that have been vapor sampled. 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 730 ppmv corresponds to less than 0.5 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank U-103 was determined to be 555 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, 555 ppmv hydrogen concentration in tank U-103 corresponds to about 1.4 % of its LFL. At this level, hydrogen is not a flammability concern in tank U-103.

The nitrous oxide concentration in tank U-103, 878 ppmv, is the highest measured in any passively ventilated tank that has been sampled. Nitrous oxide has been detected in other passively ventilated waste tanks at average concentrations as low as about 12 ppmv in tank TX-105 (Klinger et al. 1995), and as high as [763 ppmv] in tank C-103² (Huckaby and Story 1994). Under 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 U-103 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank U-103 headspace was measured in each of the 3 SUMMATM canister samples to be < 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

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

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

on carbon monoxide has varied from tank to tank. However, in waste tank headspace elevated carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks. Carbon monoxide has not been measured at very high levels in any of the waste tanks, the highest level measured to date was [26.7 ppmv] in tank C-103³ (Huckaby and Story 1994).

The carbon dioxide concentration in the tank U-103 headspace, reported as < 64 ppmv, is significantly lower than it is in ambient air. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids in the waste tanks, and converted to carbonate in solution. 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. The 2 ambient air samples collected at the start of the tank U-103 gas and vapor sampling event, for example, were measured to have an average 364 ppmv of carbon dioxide. Because different analytical methods have been used to measure carbon dioxide in the waste tank samples, the information on carbon dioxide varies. The < 64 ppmv of carbon dioxide characterization of the tank U-103 headspace is typical of that found in other passively ventilate tanks that have been sampled.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank U-103 headspace were determined to be ≤ 0.03 and ≤ 0.02 ppmv, respectively. These are acid gases that would have very low equilibrium concentrations above the high pH sludge in tank U-103. The measurable presence of nitric oxide is not uncommon in the waste tank headspaces, and 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 U-103 headspace.

The water vapor concentration of tank U-103 was determined to be about 12.2 mg/L, at the measured tank headspace temperature of 29 °C and pressure of 982 mbar (736.8 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 16.9 mbar (12.7 torr), to a dew point of 14.9 °C, and to a relative humidity of 42 %.

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

3.4 Discussion of Inorganic Gases and Vapors

Aside from water vapor, the most abundant waste constituents in the tank U-103 headspace are nitrous oxide, ammonia, and hydrogen. These have been detected in most tank headspaces sampled to date, and are usually the dominant gas species. These 3 species are each at higher than average concentrations in tank U-103.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are excellent for the methods used. Relative standard deviations range from about 0.5 % for hydrogen to about 4.4 % for water vapor. Because the precision reported depends both on sampling parameters (e.g.,

³ See preceding footnote.

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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 U-103 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. PNL and ORNL both used a gas chromatograph (GC) equipped with a mass spectrometer (MS) detector to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Ligotke et al. (1995).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank U-103. These results were produced at PNL quality assurance impact level 2. All analyses were completed 69 days after sample collection, thus exceeding by 9 days the administratively chosen 60-day holding time limit (Keller 1994). No holding time study has been done to determine the stability of organic compounds in SUMMA™ canisters in the typical chemical matrix of the waste 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.

ORNL analyzed 3 of the 12 TST tank samples, 1 of the 2 TST field blanks, and 1 of the 2 TST trip blanks. Of the 12 TST tank samples, 4 were collected with sample volumes of about 0.2 L, 4 with volumes of about 1.0 L, and 4 with volumes of about 4.0 L. Based on the observed amounts of organic vapors trapped by one of the 1.0 L sample volume TSTs, ORNL determined that the best results would be obtained from the 1.0 L samples. The 1.0 L samples were analyzed in triplicate, and the remaining 1.0 L sample was archived.

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 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 39 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 organic compounds positively identified and quantitated in SUMMA™ samples by PNL. SUMMA™ analyses were performed according to the TO-14 methodology, except for methane analysis, which was analyzed with the inorganic gases (Ligotke et al. 1995). Only 4 of the 39 TO-14 target analytes and 7 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 24 of 27 target analytes in TST samples. 1,1-Dichloroethene, butanal, and dibutyl butylphosphonate were the only TST target analytes not detected. ORNL reported the positive identification of tributyl phosphate, but it was not quantitatively measured. The tributyl phosphate concentration was estimated to be less than 0.0001 ppmv. The average concentrations of the 7 quantified target analytes, from the analysis of 3 TSTs, are given in Table 4-2. Table 4-3 lists the 14 positively identified analytes for which at least 1 sample result was outside the instrument calibration range, and consequently not quantitatively measured. Table 4-4 lists 2 analytes determined to have exceeded their ORNL practical holding times (Jenkins 1995b). Tables 4-2, 4-3, and 4-4 are mutually exclusive, so that no analyte appears in more than 1 of these tables. Data in Tables 4-3 and 4-4 should not be considered quantitative and may not be accurate 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. (1995b) describe the ORNL practical holding time study, and report the practical holding times of butanal, 1-butanol, and 2-pentanone are 1, 17, and 34 days, respectively. Because TST analyses were not completed until 37 days after sample collection (Jenkins 1995b), the results for these 3 compounds may have been affected. It is possible that 2-pentanone was not identified in the tank U-103 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.

Analysis of the TST field and trip blanks by ORNL indicated both types of TSTs were contaminated with the ORNL target analytes. In particular, the trip blank TST was determined to have very small amounts of propanone, n-dodecane, and n-tridecane, and small amounts of dichloromethane and trichlorofluoromethane. The field blank was determined to have very small amounts of dichloromethane, benzene, n-undecane, n-dodecane, n-tridecane, and 2,2,3-trimethyldecane. The field blank also had a moderate amount of 5-octadecene. No adjustment of the ORNL results has been made to account for these observations.

Both PNL and ORNL report target analyte concentrations in ppmv of analyte in dry air. To correct for the measured water vapor content of tank U-103 and obtain concentration in ppmv of analyte in moist tank air, multiply the dry-air ppmv concentrations by 0.983.

Eleven target analytes were common to both TST and SUMMA™ analyses. Table 4-5 lists these, and their reported average concentrations in TST and SUMMA™ samples. Results from these 2 sampling and analytical methods are in good agreement for propanone, propanenitrile, benzene, and toluene. As indicated in Table 4-5, ORNL reported concentrations of dichloromethane, n-butanenitrile, n-hexane, and n-heptane in TST samples are moderately higher than the SUMMA™ sample analytical detection limit, yet were not reported as being present in the SUMMA™ samples.

The largest discrepancy between the target analyte results from the 2 methods is for ethanenitrile, which was determined to be present at 0.16 ppmv in TST samples, and 0.012 ppmv in SUMMA™ samples. Except for propanenitrile, the nitriles are generally found to be higher in TST than in SUMMA™ samples. This may be due to a variety of problems, such as poor analytical recovery of nitriles from SUMMA™ samples.

The most abundant analytes in Tables 4-1 through 4-4 are 1-butanol, ethanenitrile, and propanone, each of which was measured to have an average concentration of between 0.1 and 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. Using this method, many analytes can be tentatively identified with reasonable confidence without having to inject standards of each into the GC/MS to determine their GC retention times or specific MS patterns.

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and 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 order of decreasing estimated concentration. The list of tentatively identified compounds detected in TST samples, and their estimated concentrations, is given in Table 4-7. Compounds are listed in Table 4-7 in according to the order by which they eluted chromatographically. The averages reported by ORNL in Table 4-7 are all 3-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

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

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and Ligothke et al. (1995), respectively, and should be reviewed before this data are used for decision making. Concentrations given in Tables 4-6 and 4-7 should be considered rough estimates.

4.4 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 U-103 as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

Organic vapors in the first category (those that were placed into the tank as waste) include the semivolatile straight-chain alkanes, which were used as diluents of tributyl phosphate in various plutonium extraction

processes. These alkanes (i.e., n-undecane, n-dodecane, n-tridecane, and n-tetradecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs). Though NPHs are positively identified in tank U-103, their concentrations in tank U-103 are very low compared to other NPH-rich tanks.

Tributyl phosphate is also in the category of compounds added as waste. The estimated ≤ 0.0001 ppmv of tributyl phosphate detected in TST samples by ORNL may not be representative of its headspace concentration. 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. This would result in loss of tributyl phosphate from the sampled air, and an underestimation of its actual concentration in the tank headspace. The presence of the NPHs, which were used as tributyl phosphate process diluents, and the relative abundance of 1-butanol, a known hydrolysis product of tributyl phosphate, suggest that there are small amounts of tributyl phosphate in tank U-103 waste.

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 4-9 fall into this category, including the alcohols, aldehydes, ketones, nitriles, and volatile alkanes, all of which have been associated with the degradation of the NPHs.

Though not present in high concentrations, 9 alkyl nitriles were identified in TST samples. Many nitrogen-containing cyclic compounds were also detected in TST samples, including pyridines, pyrazines, pyrazoles, and oxazoles.

On the basis of concentrations, alcohols are the dominant type of organic compounds in the tank U-103 headspace. The volatile alcohols methanol, ethanol, 1-propanol, and 2-propanol account for about 35 % by weight (wt%) of the total estimated concentration of organic compounds in TST samples. Similarly, methanol, ethanol, and 1-propanol account for about 49 wt% of the total estimated organic compound concentration in SUMMA™ samples. The abundance of volatile alcohols is similar to that found in tanks U-105, U-106, U-107, and U-111. Also similar to these other 241-U farm tanks, and in contrast to tanks having higher NPH concentrations, tank U-103 has relatively few aldehydes.

Ambient air SUMMA™ samples collected during the tank U-103 sampling event indicated low levels of propanone (i.e., 0.008 and 0.023 ppmv) and ethanenitrile (0.11 to 0.21 ppmv) in the ambient air. Methanol was also detected in the ambient air sample collected via the VSS manifold, but not when ambient air was sampled directly. This suggests that trace amounts of methanol may have existed in the VSS manifold, even after it was heated and purged with ambient air for 30 min. The reported concentration of methanol in the ambient air sample collected via the VSS manifold, 0.12 ppmv, was small compared to the estimated tank U-103 methanol concentration of 2.2 ppmv.

The total organic vapor concentration of tank U-103 was estimated by Jenkins et al. (1995a) to be about 7.2 mg/m³ from the analysis of 3 TST samples by GC/MS. A similar summation of organic compounds measured in SUMMA™ samples from tank U-103 provides an estimated total organic vapor concentration of 11 mg/m³. This disagreement is largely due to the different estimated concentrations of the dominant alcohols in the 2 sample types.

In summary, the types and concentrations of organic vapors in tank U-103 are similar to those of other 241-U farm tanks. The organic vapors in tank U-103 indicate the presence of tributyl phosphate, the semivolatile NPHs and their degradation products in the tank waste. As with the other 241-U farm tanks sampled to date, the concentrations of short-chain alcohols are higher in tank U-103 than in waste tanks with higher NPH vapor concentrations. Conversely, aldehydes are less abundant in tank U-103 than in NPH-rich waste tanks.

5.0 SUMMARY

The tank U-103 headspace was sampled in February 1995 for gases and vapors to address flammability and industrial hygiene concerns. Collection and analysis of samples has been reported. However, the measured ammonia concentration of 730 ppmv does exceed the industrial hygiene notification limit of 150 ppmv. It was determined that no other 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 U-103 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 U-103 Inorganic Gas and Vapor Concentrations -- Analyses by Pacific Northwest Laboratory

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	730	18	2.5
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	< 64	--	--
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	< 12	--	--
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	555	2.5	0.5
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.03	--	--
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	878	24	2.7
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	17,200 (12.2 mg/L)	750 (0.5 mg/L)	4.4

¹ CAS = Chemical Abstracts Service.

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

Table 4-1
Tank U-103 Quantitatively Measured Organic Compounds in SUMMA™ Sample --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (ppmv)	Standard Deviation (ppmv)	RSD ³ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.012	0.001	4
2	Propanone (acetone)	67-64-1	0.17	0.03	16
3	Trichlorofluoromethane	75-69-4	0.11	0.01	7
4	Propanenitrile	107-12-0	0.0070	0.0013	18
5	1-Propanol	71-23-8	0.034	0.013	38
6	2-Butanone	78-93-3	0.0060	0.0015	25
7	Tetrahydrofuran	109-99-9	0.034	0.002	5
8	Benzene	71-43-2	0.0053	0.0002	4
9	Tetrachloromethane (carbon tetrachloride)	56-23-5	0.0070	0.0002	3
10	Cyclohexane	110-82-7	0.024	0.001	3
11	Toluene	108-88-3	0.019	0.0004	2
12	Methane	74-82-8	< 61	--	--
Sum of positively identified compounds:			1.61	mg/m ³	

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 %.

Table 4-2
Tank U-103 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	0.16	0.01	9
2	Propanone (acetone)	67-64-1	0.14	0.01	5
3	Benzene	71-43-2	0.011	0.0004	4
4	n-Butanenitrile	109-74-0	0.016	0.002	13
5	n-Heptane	142-82-5	0.0081	0.0017	21
6	Toluene	108-88-3	0.032	0.001	4
7	n-Tridecane	629-50-5	0.0034	0.0005	15
Sum of positively identified compounds:			2.1 mg/m ³		

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

2 CAS = Chemical Abstract Service.

3 Average based on 3, 1-L samples.

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

Table 4-3
Tank U-103 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	Dichloromethane ⁵ (methylene chloride)	75-09-2	0.017	—	—
2	Propanenitrile	107-12-0	0.0092	0.0022	24
3	n-Hexane	110-54-3	0.0071	0.0008	12
4	n-Pentanenitrile	110-59-8	0.0013	0.0003	24
5	2-Hexanone	591-78-6	0.0026	0.0003	11
6	n-Octane	111-65-9	0.0027	0.0005	19
7	n-Hexanenitrile	628-73-9	0.00052	0.00008	15
8	2-Heptanone	110-43-0	0.0012	0.0002	12
9	n-Nonane	111-84-2	0.0016	0.0001	9
10	n-Heptanenitrile	629-08-3	0.00031	0.00002	7
11	2-Octanone	111-13-7	0.00050	0.00009	18
12	n-Decane	124-18-5	0.0011	0.0002	15
13	n-Undecane	1120-21-4	0.0013	0.0001	5
14	n-Dodecane	112-40-3	0.0014	0.0002	12
Sum of positively identified compounds:			2.1 mg/m ³		

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 based on 3, 1-L samples.

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

5 Dichloromethane was only detected in 2 TST samples. The 2 reported values (0.0016 and 0.032 ppmv) had a 181 relative percent difference.

Table 4-4
Tank U-103 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	0.29	0.02	6
2	2-Pentanone ⁵	107-87-9	0.0019	0.0005	27
Sum of positively identified compounds:			2.1 mg/m ³		

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

2 CAS = Chemical Abstract Service.

3 Average based on 3, 1-L samples.

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

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

Table 4-5
Tank U-103 Comparison of Organic Compounds in TST and SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory
and Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	TST ² Average (ppmv)	SUMMA™ Average ³ (ppmv)	PRD ⁴ (%)
1	1,1-Dichloroethene (vinylidene chloride)	75-35-4	< 0.0023	< 0.005	--
2	Dichloromethane (methylene chloride)	75-09-2	0.017	< 0.005	> 109
3	Propanone (acetone)	67-64-1	0.14	0.17	19
4	Ethanenitrile (acetonitrile)	75-05-8	0.16	0.012	172
5	Propanenitrile	107-12-0	0.0092	0.007	27
6	n-Butanenitrile	109-74-0	0.016	< 0.005	> 105
7	Benzene	71-43-2	0.011	0.0053	70
8	Toluene	108-88-3	0.032	0.019	51
9	n-Hexane	110-54-3	0.0071	< 0.005	> 35
10	n-Heptane	142-82-5	0.0081	< 0.005	> 47
11	n-Decane	124-18-5	0.0011	< 0.005	--

1 CAS = Chemical Abstract Service.

2 Analyses of 3, 1-L samples conducted by ORNL.

3 Analyses of 3 samples conducted by PNL.

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

Table 4-6
Tank U-103 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratories

Cmpd #	Compounds	CAS ¹ Number	Average ⁵ (mg/m ³)	Standard Deviation ² (mg/m ³)
1	Methyl Alcohol	67-56-1	3.15	0.28
2	Ethanol ³	64-17-5	2.26	--
3	1-Butanol ³	71-36-3	0.75	0.06
4	1-Butene	106-98-9	0.72	0.04
5	Unknown Alkane		0.60	0.39
6	n-Butane	106-97-8	0.50	0.20
7	Propene	115-07-1	0.36	0.02
8	Propane	74-98-6	0.36	0.03
9	Cyclopropane	75-19-4	0.19	0.04
10	Dimethyl ether	115-10-6	0.17	0.08
11	n-Pentane ⁴	109-66-0	0.13	--
12	Unknown C4 Alkene/Cycloalkane ⁴		0.13	0.01
13	N-Nitrosodimethylamine ³	62-75-9	0.045	0.005
14	Acetaldehyde	75-07-0	< 0.02	--
15	2-Butanone	78-93-3	< 0.03	--
Sum of tentatively identified compounds:			9.4	

1 CAS = Chemical Abstract Service.

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

3 Detected in only 1 sample.

4 Detected in only 2 samples.

5 Average of 3 samples, presented values are estimates.

Table 4-7
Tank U-103 Tentatively Identified Organic Compounds in TST Samples
in Order of Chromatographic Elution --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Carbon Dioxide	124-38-9	0.44	0.39
2	1-Propene, 2-methyl-	115-11-7	0.016	0.027
3	Methyl Alcohol	67-56-1	0.94	0.54
4	1-Propene, 2-methyl-	115-11-7	0.0044	0.0076
5	Methane, dichlorofluoro-	75-43-4	0.0081	0.0140
6	Ethanol	64-17-5	1.26	0.15
7	Trichloromonofluoromethane	75-69-4	0.68	0.41
8	Isopropyl Alcohol	67-63-0	0.19	0.07
9	2-Propenenitrile and 2,2-dimethylbutane		0.027	0.001
10	Pentane, 2-methyl-	107-83-5	0.033	0.004
11	1-Propanol	71-23-8	0.098	0.008
12	1-Butanol, 2-methyl-	137-32-6	0.015	0.013
13	Cyclobutanol and others		0.0059	0.0102
14	Furan, tetrahydro-	109-99-9	0.080	0.004
15	2-Propanone, 1,1,1-trifluoro-	421-50-1	0.017	0.030
16	1-Propanol, 2-methyl	78-83-1	0.0054	0.0093
17	Acetic acid, methyl ester	79-20-9	0.047	0.081
18	1,2,3,6-tetrahydropyridine	694-05-3	0.013	0.011
19	1,4-Dioxane	123-91-1	0.018	0.006
20	Pyrazine	290-37-9	0.19	0.01
21	Methyl Isobutyl Ketone	108-10-1	0.028	0.004
22	Propane, 2-methyl-2-nitro-	594-70-7	0.032	0.005
23	N-Nitrosodimethyl-amine	62-75-9	0.21	0.02
24	Formamide and others		0.019	0.017
25	Heptane, 3-methyl-	589-81-1	0.0037	0.0064
26	1H-1,2,4-Triazole	288-88-0	0.0089	0.0154

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	1-Octene	111-66-0	0.0048	0.0083
28	Cyclopropane, (1-methylethyl)-	3638-35-5	0.033	0.029
29	Tetrachloroethylene	127-18-4	0.022	0.001
30	Cyclotrisiloxane, hexamethyl	541-05-9	0.023	0.030
31	Pyrazine, methyl-	109-08-0	0.014	0.002
32	Oxazole, 4,5- dihydro-2-methyl-	1120-64-5	0.026	0.007
33	Ethylbenzene	100-41-4	0.020	0.002
34	p-Xylene	106-42-3	0.067	0.005
35	Pyridine, 3-methyl-	108-99-6	0.0057	0.0098
36	3-Heptanone	106-35-4	0.019	0.002
37	p-Xylene	106-42-3	0.029	0.002
38	Pyrazine, ethyl-	13925-00-3	0.0078	0.0069
39	3-Hexenal, (Z)-	6789-80-6	0.021	0.003
40	Cyclohexane, octyl	1795-15-9	0.013	0.002
41	2-Hexenoic acid, 4-methylphenyl ester	69687-91-8	0.013	0.002
42	2-Heptanone, 6-methyl-	928-68-7	0.0034	0.0060
43	1-Decene	872-05-9	0.044	0.005
44	Phenol and cyclotetrasiloxane, octamethyl		0.023	0.011
45	Benzene, tert-butyl-	98-06-6	0.024	0.002
46	1-Heptanol	111-70-6	0.011	0.002
47	1-Hexanol, 2-ethyl-	104-76-7	0.014	0.002
48	Nonanenitrile	2243-27-8	0.0081	0.0078
49	1H-Pyrazole, 4,5- dihydro-5-propyl-	75011-90-4	0.0076	0.0131
50	Oxazole, 4,5- dimethyl-2-propyl-	53833-32-2	0.033	0.003
51	Formamide, n-butyl and others		0.019	0.009
52	Benzyl Alcohol	100-51-6	0.0078	0.0136
53	alkyl nitrile		0.0034	0.0059
54	Acetophenone	98-86-2	0.0058	0.0051

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	4(1H)-Pyrimidinone and others		0.0022	0.0039
56	Undecane, 4,4-dimethyl-	17312-68-4	0.024	0.003
57	Naphthalene and others		0.010	0.001
58	2-Oxazolidinone, 5-methyl-3-(2-propenyl)-	55956-20-2	0.020	0.003
59	Decane, 5-propyl-	17312-62-8	0.0024	0.0041
60	Dodecane, 2,7,10-trimethyl-	74645-98-0	0.0047	0.0041
61	Tetradecane	629-59-4	0.012	0.001
62	Hexadecanoic acid	57-10-3	0.0056	0.0051
63	Tetradecanoic acid	544-63-8	0.0073	0.0127
64	Benzenesulfonamide, N-butyl	3622-84-2	0.045	0.008
65	Isopropyl Palmitate	142-91-6	0.031	0.029
Sum of tentatively identified compounds:			5.07	

1 CAS = Chemical Abstract Service.

2 Average based on 3, 1-L samples, presented values are estimates.

Table 4-8
 Tank U-103 Tentatively Identified Organic Compounds in TST Samples --
 Sorted Alphanumerically
 Analyses by Oak Ridge National Laboratories

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
43	1-Decene	872-05-9	0.044	0.005
2	1-Propene, 2-methyl-	115-11-7	0.016	0.027
27	1-Octene	111-66-0	0.0048	0.0083
4	1-Propene, 2-methyl-	115-11-7	0.0044	0.0076
46	1-Heptanol	111-70-6	0.011	0.002
16	1-Propanol, 2-methyl	78-83-1	0.0054	0.0093
47	1-Hexanol, 2-ethyl-	104-76-7	0.014	0.002
12	1-Butanol, 2-methyl-	137-32-6	0.015	0.013
11	1-Propanol	71-23-8	0.098	0.008
19	1,4-Dioxane	123-91-1	0.018	0.006
18	1,2,3,6-tetrahydro- pyridine	694-05-3	0.013	0.011
26	1H-1,2,4-Triazole	288-88-0	0.0089	0.0154
49	1H-Pyrazole, 4,5- dihydro-5-propyl-	75011-90-4	0.0076	0.0131
41	2-Hexenoic acid, 4-methylphenyl ester	69687-91-8	0.013	0.002
15	2-Propanone, 1,1,1-trifluoro-	421-50-1	0.017	0.030
42	2-Heptanone, 6-methyl-	928-68-7	0.0034	0.0060
58	2-Oxazolidinone, 5-methyl-3-(2-propenyl)-	55956-20-2	0.020	0.003
9	2-Propenenitrile and 2,2-dimethylbutane		0.027	0.001
36	3-Heptanone	106-35-4	0.019	0.002
39	3-Hexenal, (Z)-	6789-80-6	0.021	0.003
55	4(1H)-Pyrimidinone and others		0.0022	0.0039
17	Acetic acid, methyl ester	79-20-9	0.047	0.081
54	Acetophenone	98-86-2	0.0058	0.0051
53	alkyl nitrile		0.0034	0.0059
45	Benzene, tert-butyl-	98-06-6	0.024	0.002

WHC-SD-WM-ER-510 REV. 0

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
64	Benzenesulfonamide, N-butyl	3622-84-2	0.045	0.008
52	Benzyl Alcohol	100-51-6	0.0078	0.0136
1	Carbon Dioxide	124-38-9	0.44	0.39
13	Cyclobutanol and others		0.0059	0.0102
40	Cyclohexane, octyl	1795-15-9	0.013	0.002
28	Cyclopropane, (1-methylethyl)-	3638-35-5	0.033	0.029
30	Cyclotrisiloxane, hexamethyl	541-05-9	0.023	0.030
59	Decane, 5-propyl-	17312-62-8	0.0024	0.0041
60	Dodecane, 2,7,10-trimethyl-	74645-98-0	0.0047	0.0041
6	Ethanol	64-17-5	1.26	0.15
33	Ethylbenzene	100-41-4	0.020	0.002
24	Formamide and others		0.019	0.017
51	Formamide, n-butyl and others		0.019	0.009
14	Furan, tetrahydro-	109-99-9	0.080	0.004
25	Heptane, 3-methyl-	589-81-1	0.0037	0.0064
62	Hexadecanoic acid	57-10-3	0.0056	0.0051
8	Isopropyl Alcohol	67-63-0	0.19	0.07
65	Isopropyl Palmitate	142-91-6	0.031	0.029
5	Methane, dichlorofluoro-	75-43-4	0.0081	0.0140
3	Methyl Alcohol	67-56-1	0.94	0.54
21	Methyl Isobutyl Ketone	108-10-1	0.028	0.004
23	N-Nitrosodimethyl-amine	62-75-9	0.21	0.02
57	Naphthalene and others		0.010	0.001
48	Nonanenitrile	2243-27-8	0.0081	0.0078
32	Oxazole, 4,5- dihydro-2-methyl-	1120-64-5	0.026	0.007
50	Oxazole, 4,5- dimethyl-2-propyl-	53833-32-2	0.033	0.003
34	p-Xylene	106-42-3	0.067	0.005
37	p-Xylene	106-42-3	0.029	0.002
10	Pentane, 2-methyl-	107-83-5	0.033	0.004

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
44	Phenol and cyclotetrasiloxane, octamethyl		0.023	0.011
22	Propane, 2-methyl-2-nitro-	594-70-7	0.032	0.005
20	Pyrazine	290-37-9	0.19	0.01
31	Pyrazine, methyl-	109-08-0	0.014	0.002
38	Pyrazine, ethyl-	13925-00-3	0.0078	0.0069
35	Pyridine, 3-methyl-	108-99-6	0.0057	0.0098
29	Tetrachloroethylene	127-18-4	0.022	0.001
61	Tetradecane	629-59-4	0.012	0.001
63	Tetradecanoic acid	544-63-8	0.0073	0.0127
7	Trichloromonofluoromethane	75-69-4	0.68	0.41
56	Undecane, 4,4-dimethyl-	17312-68-4	0.024	0.003
Sum of tentatively identified compounds:			5.07	

1 CAS = Chemical Abstract Service.

2 Average based on 3, 1-L samples, presented values are estimates.

Table 4-9
 Tank U-103 Tentatively Identified Organic Compounds in TST Samples --
 Sorted by Estimated Concentration
 Analyses by Oak Ridge National Laboratory.

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
6	Ethanol	64-17-5	1.26	0.15
3	Methyl Alcohol	67-56-1	0.94	0.54
7	Trichloromonofluoromethane	75-69-4	0.68	0.41
1	Carbon Dioxide	124-38-9	0.44	0.39
23	N-Nitrosodimethyl-amine	62-75-9	0.21	0.02
20	Pyrazine	290-37-9	0.19	0.01
8	Isopropyl Alcohol	67-63-0	0.19	0.07
11	1-Propanol	71-23-8	0.098	0.008
14	Furan, tetrahydro-	109-99-9	0.080	0.004
34	p-Xylene	106-42-3	0.067	0.005
17	Acetic acid, methyl ester	79-20-9	0.047	0.081
64	Benzenesulfonamide, N-butyl	3622-84-2	0.045	0.008
43	1-Decene	872-05-9	0.044	0.005
10	Pentane, 2-methyl-	107-83-5	0.033	0.004
28	Cyclopropane, (1-methylethyl)-	3638-35-5	0.033	0.029
50	Oxazole, 4,5- dimethyl-2-propyl-	53833-32-2	0.033	0.003
22	Propane, 2-methyl-2-nitro-	594-70-7	0.032	0.005
65	Isopropyl Palmitate	142-91-6	0.031	0.029
37	p-Xylene	106-42-3	0.029	0.002
21	Methyl Isobutyl Ketone	108-10-1	0.028	0.004
9	2-Propenenitrile and 2,2-dimethylbutane		0.027	0.001
32	Oxazole, 4,5- dihydro-2-methyl-	1120-64-5	0.026	0.007
56	Undecane, 4,4-dimethyl-	17312-68-4	0.024	0.003
45	Benzene, tert-butyl-	98-06-6	0.024	0.002
44	Phenol and cyclotetrasiloxane, octamethyl		0.023	0.011

WHC-SD-WM-ER-510 REV. 0

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
30	Cyclotrisiloxane, hexamethyl	541-05-9	0.023	0.030
29	Tetrachloroethylene	127-18-4	0.022	0.001
39	3-Hexenal, (Z)-	6789-80-6	0.021	0.003
58	2-Oxazolidinone, 5-methyl-3-(2-propenyl)-	55956-20-2	0.020	0.003
33	Ethylbenzene	100-41-4	0.020	0.002
24	Formamide and others		0.019	0.017
36	3-Heptanone	106-35-4	0.019	0.002
51	Formamide, n-butyl and others		0.019	0.009
19	1,4-Dioxane	123-91-1	0.018	0.006
15	2-Propanone, 1,1,1-trifluoro-	421-50-1	0.017	0.030
2	1-Propene, 2-methyl-	115-11-7	0.016	0.027
12	1-Butanol, 2-methyl-	137-32-6	0.015	0.013
31	Pyrazine, methyl-	109-08-0	0.014	0.002
47	1-Hexanol, 2-ethyl-	104-76-7	0.014	0.002
40	Cyclohexane, octyl	1795-15-9	0.013	0.002
41	2-Hexenoic acid, 4-methylphenyl ester	69687-91-8	0.013	0.002
18	1,2,3,6-tetrahydro- pyridine	694-05-3	0.013	0.011
61	Tetradecane	629-59-4	0.012	0.001
46	1-Heptanol	111-70-6	0.011	0.002
57	Naphthalene and others		0.010	0.001
26	1H-1,2,4-Triazole	288-88-0	0.0089	0.0154
5	Methane, dichlorofluoro-	75-43-4	0.0081	0.0140
48	Nonanenitrile	2243-27-8	0.0081	0.0078
38	Pyrazine, ethyl-	13925-00-3	0.0078	0.0069
52	Benzyl Alcohol	100-51-6	0.0078	0.0136
49	1H-Pyrazole, 4,5- dihydro-5-propyl-	75011-90-4	0.0076	0.0131
63	Tetradecanoic acid	544-63-8	0.0073	0.0127
13	Cyclobutanol and others		0.0059	0.0102

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
54	Acetophenone	98-86-2	0.0058	0.0051
35	Pyridine, 3-methyl-	108-99-6	0.0057	0.0098
62	Hexadecanoic acid	57-10-3	0.0056	0.0051
16	1-Propanol, 2-methyl	78-83-1	0.0054	0.0093
27	1-Octene	111-66-0	0.0048	0.0083
60	Dodecane, 2,7,10-trimethyl-	74645-98-0	0.0047	0.0041
4	1-Propene, 2-methyl-	115-11-7	0.0044	0.0076
25	Heptane, 3-methyl-	589-81-1	0.0037	0.0064
53	alkyl nitrile		0.0034	0.0059
42	2-Heptanone, 6-methyl-	928-68-7	0.0034	0.0060
59	Decane, 5-propyl-	17312-62-8	0.0024	0.0041
55	4(1H)-Pyrimidinone and others		0.0022	0.0039
Sum of tentatively identified compounds:			5.07	

1 CAS = Chemical Abstract Service.

2 Average based on 3, 1-L samples, presented values are estimates.

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