~~XXXX~~ RMIS View/Print Document Cover Sheet ~~XXXX~~

This document was retrieved from the Boeing ISEARCH System.

Accession #: D196054782

Document #: SD-WM-ER-446

Title/Desc:

TANK 241S102 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
3/1995

COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 2

1. ECN 626287

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-S-102 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN MARCH 1995	6. Bldg./Sys./Fac. No. 2704HV/200E	7. Approval Designator N/A
	8. Document Numbers Changed by this ECN (includes sheet no. and rev.) WHC-SD-WM-ER-446 REV <u>XO 9/28/95</u> <i>KMB</i>	9. Related ECN No(s). N/A	10. Related PO No. 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 <u>19</u> BY WHC DATE SEP 27 1995 <i>Sta. 11</i>	

ENGINEERING CHANGE NOTICE

Page 2 of 2

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

626287

15. Design Verification Required	16. Cost Impact				17. Schedule Impact (days)
	ENGINEERING		CONSTRUCTION		
	Additional	☐ \$	Additional	☐ \$	
☐ Yes	Savings	☐ \$	Savings	☐ \$	Improvement ☐
☒ No					Delay ☐

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

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

19. Other Affected Documents: (NOTE: Documents listed below will not be revised by this ECN.) Signatures below indicate that the signing organization has been notified of other affected documents listed below.

Document Number/Revision

Document Number/Revision

Document Number Revision

20. Approvals

Signature	Date	Signature	Date
<u>OPERATIONS AND ENGINEERING</u>		<u>ARCHITECT-ENGINEER</u>	
Cog. Eng. D. R. Bratzel <i>DR Bratzel</i>	<i>9/25/95</i>	PE	
Cog. Mgr. T. J. Kelley <i>TJ Kelley</i>	<i>9/25/95</i>	QA	
QA		Safety	
Safety		Design	
Environ.		Environ.	
Other		Other	
Proj.			
Proj.			
Proj.			
Proj.			
		<u>DEPARTMENT OF ENERGY</u>	
		Signature or a Control Number that tracks the Approval Signature	
		<u>ADDITIONAL</u>	

SEP 27 1995

RELEASE AUTHORIZATION

Document Number: WHC-SD-WM-ER-446, REV 1

Document Title: Tank 241-S-102 Headspace Gas and Vapor
Characterization Results for Samples Collected in
March 1995

Release Date: 9/26/95

**This document was reviewed following the
procedures described in WHC-CM-3-4 and is:**

APPROVED FOR PUBLIC RELEASE

WHC Information Release Administration Specialist:

Kara Broz

9/26/95

TRADEMARK DISCLAIMER. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors.

This report has been reproduced from the best available copy. Available in paper copy. Printed in the United States of America. To obtain copies of this report, contact:

Westinghouse Hanford Company - Document Control Services
P.O. Box 1970, Mailstop H6-08, Richland, WA 99352
Telephone: (509) 372-2420; Fax: (509) 376-4989

SUPPORTING DOCUMENT

1. Total Pages *31*

2. Title

TANK 241-S-102 HEADSPACE GAS AND VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
MARCH 1995

3. Number

WHC-SD-WM-ER-446

4. Rev No.

1

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

OFFICIAL RELEASE *19*
BY WHC
DATE
Stand SEP 27 1995

[illegible]

Tank 241-S-102 Headspace Gas and Vapor Characterization Results for Samples Collected in March 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

Contents

1.0 INTRODUCTION	1
1.1 Characterization Objectives	1
1.2 Characterization Data Criteria	1
1.3 Sampling Overview	2
1.4 Tank Headspace Dynamics	2
2.0 SAMPLING EVENT	3
3.0 INORGANIC GASES AND VAPORS	4
3.1 Ammonia, Hydrogen, and Nitrous Oxide	4
3.2 Carbon Monoxide and Carbon Dioxide	5
3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium	5
3.4 Discussion of Inorganic Gases and Vapors	6
4.0 ORGANIC VAPORS	7
4.1 Positively Identified Organic Compounds	7
4.2 Tentatively Identified Organic Compounds	8
4.3 Discussion of Organic Compounds	9
5.0 SUMMARY	11
6.0 REFERENCES	12

Acronyms and Abbreviations

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

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-S-102 Headspace Gas and Vapor Characterization Results
for Samples Collected in March 1995

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank S-102 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). The tank S-102 headspace was 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 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 single shell Watchlist waste tanks, such as tank S-102, 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 S-102 headspace characterization data presented here are from a single sampling event. Samples collected are thought to have been representative of the tank headspace when the tank was sampled (Meacham et al. 1995), and sample analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents. No assessment has been made of how the tank S-102 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 S-102 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

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

The cascade of tanks S-101, S-102, and S-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 S-102 using the vapor sampling system (VSS) on March 14, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-S-102 Tank Characterization Plan* (Homi 1995a). The tank headspace temperature was determined to be 24.3 °C. Air from the tank S-102 headspace was withdrawn from a single elevation via a 6.1-m long heated sampling probe mounted in riser 1, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C. All tank air samples were collected between 11:26 a.m. and 2:47 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 3-1 by analytical laboratory. Table 3-1 also lists the 14 trip blanks and 2 field blanks provided by the laboratories.

A general description of vapor sampling and sample analysis methods is given by Huckaby and Babad (1995). The sampling equipment, sample collection sequence, sorbent trap sample air flow rates and flow times, chain of custody information, and a discussion of the sampling event itself are given in WHC (1995b).

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,1} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions as given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM canisters were prepared and analyzed by PNL (Pool et al. 1995). All sample preparation and analyses were performed at PNL quality assurance impact level 2.

Analyses of SUMMATM canisters and sorbent traps for inorganic compounds were performed 64 and 30 days, respectively, after sample collection (Ligothke 1995). Sorbent trap analyses were within the specified 60-day maximum holding time allowed by the WHC quality assurance project plan (Keller 1994), however, the SUMMATM canister analyses exceeded the 60-day holding time. The 60-day allowed holding time was administratively chosen, because no holding time study has been performed to address the stability of compounds in SUMMATM canisters in the chemical matrix of the tank samples. 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 though the 60-day holding time limit was exceeded.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 412 ppmv, is relatively high compared to other waste tanks sampled to date. 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 412 ppmv corresponds to about 0.3% of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank S-102 was determined to be 669 ppmv, and is among the highest measured in any of the passively ventilated waste tanks. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, the 669 ppmv hydrogen concentration in tank S-102 corresponds to about 1.7 % of its LFL. At this level, hydrogen is not a flammability concern in tank S-102.

The nitrous oxide concentration in tank S-102, 509 ppmv, is also relatively high compared to other waste tanks sampled to date. 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 868 ppmv in tank U-103 (Ligothke et al. 1995). Under the proper conditions, nitrous oxide can serve as an oxidizer to support combustion. However, Cashdollar et al. (1992) found that nitrous oxide had no significant effect on the flammability of hydrogen and air mixtures for hydrogen concentrations less than 20 vol%, and that "small amounts of nitrous oxide (relative to air) do not appear to have much effect on the flammability". Their results suggest the measured nitrous oxide concentration is much too low to have a significant effect on the flammability of the tank S-102 headspace.

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

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank S-102 headspace was measured as < 12 ppmv. In ambient air it typically ranges from 0.05 to 0.15 ppmv. Because different analytical methods have been used to measure carbon monoxide in the waste tanks sampled to date, the information on carbon monoxide has varied from tank to tank. However, elevated waste tank headspace carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks. 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-103² (Huckaby and Story 1994).

The carbon dioxide concentration in the tank S-102 headspace, reported as < 64 ppmv, is significantly lower than it is in ambient air. Carbon dioxide is normally present in the ambient air at a concentration of 350 to 400 ppmv, and is typically lower than ambient in the waste tank headspaces. The 2 ambient air samples collected at the start of the tank S-102 gas and vapor sampling event, for example, were measured to have an average 360 ppmv of carbon dioxide.

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. Like the carbon monoxide measurements, because different analytical methods have been used to measure carbon dioxide in the waste tank samples, the information on waste tank carbon dioxide varies. The < 64 ppmv of carbon dioxide characterization of the tank S-102 headspace is consistent with typical values for the waste tanks sampled to date.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank S-102 headspace were determined to be ≤ 0.04 and ≤ 0.02 ppmv, respectively. These are acid gases that would have very low equilibrium concentrations above the high pH sludge in tank S-102. A 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 S-102 headspace.

The water vapor concentration of tank S-102 was determined to be about 14.1 mg/L, at the measured tank headspace temperature of 24.3 °C and pressure of 988.0 mbar (741.2 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 19.3 mbar (14.5 torr), to a dew point of 16.9 °C, and to a relative humidity of 63 %.

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).

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

3.4 Discussion of Inorganic Gases and Vapors

Aside from water vapor, the most abundant waste constituents in the tank S-102 headspace are hydrogen, nitrous oxide, and ammonia. These have been detected in most tank headspaces sampled to date, and are usually the dominate waste species. The concentrations of these 3 constituents in tank S-102 are well above the average measured in passively ventilated waste tanks.

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 less than 1 % for hydrogen to about 7 % for nitrous oxide results. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), small relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

4.0 ORGANIC VAPORS

Organic vapors in the tank S-102 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Gas chromatographs (GCs) equipped with mass spectrometer (MS) detectors were used by PNL and ORNL to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Pool et al. (1995).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank S-102. PNL results were produced at PNL quality assurance impact level 2. All PNL analyses were completed 21 days after sample collection (Ligotke 1995), and were within the administratively chosen 60-day maximum holding time (Keller 1994). However, 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. 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 by analysis of standards. The concentration of an analyte in the sample is said to be quantitatively measured if the response of the GC/MS has been established at several known concentrations of that analyte (i.e., the GC/MS has been calibrated for that analyte), and the MS response to the analyte in the sample is between the lowest and highest responses to the known concentrations (i.e., the analyte is within the calibration range).

ORNL and PNL were assigned different lists of organic compounds, or target analytes, to positively identify and measure quantitatively. The ORNL target analyte list was derived from a review of the tank C-103 headspace constituents by a panel of toxicology experts (Mahlum et al. 1994). The PNL target analyte list included 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. SUMMA™ analyses were performed according to the TO-14 methodology, except for methane analysis, which was analyzed with the inorganic gases (Pool et al. 1995). Only 5 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. Dichloromethane, dibutyl butylphosphonate, and tributyl phosphate were the only TST target analytes not detected. The positively identified organic compounds and their average concentrations from the analyses of 3 TSTs are listed in Tables 4-2, 4-3, and 4-4. Table 4-2 lists 11 compounds which were quantitated. Table 4-3 lists 10 compounds for which the measured amount in at least 1 TST sample was outside of the instrument calibration (and consequently were not quantitated). Table 4-4 lists 3 compounds for which the analyte-specific ORNL practical holding time was exceeded. 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 may not be accurate to within $\pm 30\%$ as specified by Burnum (1995).

The ORNL practical holding time is defined as the holding time for which there is a 15 % risk that the concentration of an analyte in the sample will be below its initial concentration. As indicated in Table 4-4, of butanal, 1-butanol, and 2-pentanone exceeded their practical holding times, and may have been affected by the 36 day period between sample collection and analysis (Jenkins 1995b). Jenkins et al (1995b) describe the ORNL practical holding time study, and report practical holding times for butanal, 1-butanol, and 2-pentanone to be 1, 17, and 34 days, respectively. It should be noted that the contractual holding time for the TST samples was 60 days.

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 S-102 and obtain concentration in ppmv of analyte in moist tank air, multiply the dry-air ppmv concentrations by 0.981.

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

The largest discrepancy between the target analyte results from the 2 methods is for propanone, which was determined to be present at 0.10 ppmv in TST samples, and 0.56 ppmv in SUMMATM samples. Ethanenitrile and toluene measurements from the 2 types of samples differ by about a factor of 2. None of these compounds, however, even assuming the higher concentrations to be correct, are at or above levels of concern.

The most abundant analytes in Tables 4-1 through 4-4 are propanone, 1-butanol, 1-propanol, and toluene, each of which was measured to 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 these methods, 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 list of tentatively identified compounds recovered from SUMMA™ samples, with estimated concentrations, is given in Table 4-6. Compounds are listed in Table 4-6 in the order by which they eluted chromatographically, and only non-zero results are included in the reported averages. 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 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 in both Table 4-6 and 4-7 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. (1995a) and Pool et al. (1995), respectively, and should be reviewed before this data is used for decision making. Concentrations given in Tables 4-6 and 4-7 should be considered rough estimates.

4.3 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables 4-1 through 4-7 is to separate them into 2 categories: 1) Organic compounds added to tank S-102 as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

The first category encompasses all organic compounds that were placed into the tank as waste. It includes the semivolatile 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, n-tetradecane, and n-pentadecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs). Though NPHs are positively identified in tank S-102, their concentrations are very low compared to other NPH-rich tanks in the 241-BY and 241-C farms.

The tentatively identified cyclosiloxanes (i.e., Cmpd # 15 and 18 in Table 4-7), and other silicon-containing compounds (i.e., Cmpd # 9, 16, and 22 in Table 4-7) are also in this category. Small quantities of organosilicon compounds may have been introduced to the waste tank through their use as defoaming agents, but they may also be present in the headspace due to their use in liquid traps at the tank's breather riser.

The absence of tributyl phosphate in the tank S-102 samples does not necessarily indicate it is not present in the waste. The identification of the tributyl phosphate diluents and their degradation products is reason to expect tributyl phosphate may be present in the tank waste. 1-Butanol, which is one of the more abundant compounds in tank S-102 samples, is known to be a product of the hydrolysis of tributyl phosphate. Furthermore, informal tests by ORNL indicate that tributyl phosphate is adsorbed by the glass

fiber filters used during sampling to protect the samples from radiolytic particulate contamination. Based on these considerations, the lack of tributyl phosphate in the tank S-102 headspace samples should not be taken as proof it is not present in the headspace.

The second category includes all organic compounds that have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables 4-1 through 4-7 fall into this category, including the alcohols, ketones, nitriles, alkenes, and volatile alkanes, all of which have been associated with the degradation of the NPHs.

On the basis of concentration, alcohols are the dominate type of organic compound in the tank S-102 headspace. Methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, and 2-butanol account for about 76 % of the total estimated concentration of organic compounds in SUMMA™ samples. Similarly, about 65 % of the total estimated organic compound concentration in TST samples is due to the same 6 alcohols. By contrast, the NPH-rich waste tanks in 241-BY and 241-C farms have few alcohols other than 1-butanol. Also in contrast to tanks having higher NPH concentrations, tank S-102 has relatively few ketones, and no aldehydes were detected.

The total organic vapor concentration of tank S-102 was estimated by Jenkins et al. to be about 9.4 mg/m³ from the analysis of 3 TST samples by GC/MS. A similar summation of organic compounds measured in SUMMA™ samples from tank S-102 provides an estimated total organic vapor concentration of 20.6 mg/m³. This disagreement is largely due to the different estimated concentrations of the dominant alcohols in the 2 sample types.

The organic vapor concentrations in tank S-102 are moderately low. The organic vapors in tank S-102 clearly indicate the presence of the semivolatile NPHs and their degradation products in the tank waste, though the NPHs are at trace levels. Tributyl phosphate was not detected in any of the headspace samples, but there is strong evidence that it is also present in the waste. Tank S-102 is the only 241-S farm tank to be sampled to date. Its headspace organic vapor composition is quite similar to the 241-U farm tanks U-106, U-107, and U-111, in that NPH vapors are present but only in trace amounts, and the short-chain alcohols are the most abundant organic compounds.

5.0 SUMMARY

The tank S-102 headspace was sampled in March 1995 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 notification limits, but that ammonia, at 412 ppmv, did exceed the industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995b).

6.0 REFERENCES

- 29 CFR 1910.120, 1993, "Hazardous Waste Operations and Emergency Response", *Code of Federal Regulations*.
- Burnum, S. T., 1995, *Qualification of Reported WHC Vapor Program Data*, (letter 95-CHD-065 to president, Westinghouse Hanford Company, August 18), Department of Energy, Richland Operations Office, Richland, Washington.
- Cashdollar, K. L., M. Hertzberg, I. A. Zlochower, C. E. Lucci, G. M. Green, and R. A. Thomas, 1992, *Laboratory Flammability Studies of Mixtures of Hydrogen, Nitrous Oxide, and Air*, WHC-SD-WM-ES-219 Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Dougherty, L. F., 1995, *Single Shell Tank Interim Operational Safety Requirements*, WHC-SD-WM-OSR-005 Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- EPA 1988, *Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air*, PB90-127374, U.S. Environmental Protection Agency, Washington, D.C.
- EPA 1992, *Test Methods for Evaluating Solid Waste*, SW-846 Rev. 1, U.S. Environmental Protection Agency, Washington, D.C.
- Hendrickson, R. W., 1995, *Tank Vapor Characterization Oak Ridge National Laboratories Quality Assurance Assessment*, TWRSQA-95-0012, Westinghouse Hanford Company, Richland, Washington.
- Homi, C. S., 1995a, *Tank 241-S-102 Tank Characterization Plan*, WHC-SD-WM-TP-238 Rev. 0A, Westinghouse Hanford Company, Richland, Washington.
- Homi, C. S., 1995b, *Vapor Sampling and Analysis Plan*, WHC-SD-WM-TP-335 Rev. 0G, Westinghouse Hanford Company, Richland, Washington.
- Huckaby, J. L., 1994, *Tank 241-C-103 Headspace Flammability*, WHC-EP-0734 Rev. 1, Westinghouse Hanford Company, Richland, Washington.
- Huckaby, J. L., H. Babad, and D. R. Bratzel, 1995, *Headspace Gas and Vapor Characterization Summary for the 43 Vapor Program Suspect Tanks*, WHC-SD-WM-ER-514 Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Huckaby, J. L., and M. S. Story, 1994, *Vapor Characterization of Tank 241-C-103*, WHC-EP-0780 Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Jenkins, R. A., 1995a, *Untitled*, (Letter 090195A to D. Bratzel, September 1), Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- Jenkins, R. A., 1995b, *Untitled*, (Letter 091495A to D. Bratzel, September 14), Oak Ridge National Laboratory, Oak Ridge, Tennessee.

- Jenkins, R. A, A. B. Dindal, C. Y. Ma, M. A. Palausky, J. T. Skeen, and C. K. Bayne, 1995a, *Analysis of Tank 241-S-102 Headspace Components*, ORNL-CASD-FR-241S102.95 Rev. 0, Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- Jenkins, R. A, A. B. Dindal, C. Y. Ma, M. A. Palausky, J. T. Skeen, and C. K. Bayne, 1995b, *Analysis of Tank 241-TY-104 Headspace Components*, ORNL-CASD-FR-241TY104.95 Rev. 1, Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- Keller, K. K., 1994, *Quality Assurance Project Plan for Tank Vapor Characterization*, WHC-SD-WM-QAPP-013 Rev. 2, Westinghouse Hanford Company, Richland, Washington.
- Klinger, G. S., T. W. Clauss, M. W. Ligothke, K. H. Pool, R. B. Lucke, B. D. McVeety, O. P. Bredt, J. S. Young, M. McCulloch, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-TX-105: Results from Samples Collected Through the Vapor Sampling System on 12/20/94*, PNL-10594 UC-606, Pacific Northwest Laboratory, Richland, Washington.
- Ligothke, M. W., 1995, *PNL Vapor Project Analytical Holding Times*, (Letter to D.R. Bratzel, September 23, 1995), Pacific Northwest Laboratories, Richland, Washington.
- Ligothke, M. W., K. H. Pool, T. W. Clauss, B. D. McVeety, G. S. Klinger, K. B. Olsen, O. P. Bredt, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-U-103: Results from Samples Collected on 2/15/95*, PNL-10813 UC-606, Pacific Northwest Laboratory, Richland, Washington.
- Lucke, R. B., M. W. Ligothke, K. H. Pool, T. W. Clauss, A. K. Sharma, B. D. McVeety, M. McCulloch, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-C-108: Results from Samples Collected Through the Vapor Sampling System on 8/5/94*, PNL-10351 UC-606, Pacific Northwest Laboratory, Richland, Washington.
- Mahlum, D. D., J. Y. Young, and R. E. Weller, 1994, *Toxicologic Evaluation of Analytes from Tank 231-C-103*, PNL-10189, Pacific Northwest Laboratory, Richland, Washington.
- McVeety, B. D., T. W. Clauss, M. W. Ligothke, K. H. Pool, R. B. Lucke, G. S. Klinger, J. S. Young, M. McCulloch, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-BY-108: Results from Samples Collected on 10/27/94*, PNL-10495 UC-606, Pacific Northwest Laboratory, Richland, Washington.
- NFPA 1992, *Standard on Explosion Prevention Systems*, NFPA 69, National Fire Protection Association, Quincy, Massachusetts.
- Osborne, J. W., and J. L. Huckaby, 1994, *Program Plan for the Resolution of Tank Vapor Issues*, WHC-EP-0562 Rev. 1, Westinghouse Hanford Company, Richland, Washington.
- Osborne, J. W., J. L. Huckaby, T. P. Rudolph, E. R. Hewitt, D. D. Mahlum, J. Y. Young, C. M. Anderson, 1994, *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution*, WHC-SD-WM-DQO-002, Westinghouse Hanford Company, Richland, Washington.
- Pool, K. H, R. B. Lucke, B. D. McVeety, G. S. Klinger, T. W. Clauss, M. W. Ligothke, K. B. Olsen, O. P. Bredt, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-*

WHC-SD-WM-ER-446 REV. 1

S-102: Results from Samples Collected on 3/14/95, PNL-10587 UC-606, Pacific Northwest Laboratory, Richland, Washington.

WHC 1995a, Operating Specifications for Watchlist Tanks, OSD-T-151-00030, Rev. B-9, Westinghouse Hanford Company, Richland, Washington.

WHC 1995b, Vapor and Gas Sampling of Single-Shell Tank 241-S-102 Using the Vapor Sampling System, WHC-SD-WM-RPT-142, Westinghouse Hanford Company, Richland, Washington.

Table 2-1
Tank S-102 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 S-102 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	412	5	1.2
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	669	1	0.2
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.04	--	--
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	509	35	7
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	19,500 (14.1 mg/L)	400 (0.3 mg/L)	2

¹ CAS = Chemical Abstracts Service.

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

Table 4-1
Tank S-102 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	Ethanenitrile (acetonitrile)	75-05-8	0.039	0.004	12
2	Propanone (acetone)	67-64-1	0.56	0.01	1
3	Trichlorofluoromethane	75-69-4	0.034	0.002	5
4	Propanol	71-23-8	0.20	0.22	113
5	2-Butanone	78-93-3	0.080	0.018	22
6	Tetrahydrofuran	109-99-9	0.052	0.002	3
7	Benzene	71-43-2	0.019	0.0005	3
8	n-Heptane	142-82-5	0.012	0.0003	2
9	Pyridine	110-86-1	0.023	0.018	77
10	Toluene	108-88-3	0.20	0.004	2
11 & 12	para-Xylene and meta-Xylene ⁴	106-42-3 108-38-3	0.006	0.0002	3
13	Methane	74-82-8	< 12	--	--
Sum of positively identified compounds:			3.76	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 %.

4 m-xylene and p-xylene coelute and the reported value represents the sum of their concentrations.

Table 4-2
Tank S-102 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	0.081	0.014	18
2	Propanone (acetone)	67-64-1	0.10	0.02	23
3	n-Hexane	110-54-3	0.0071	0.0004	5
4	Benzene	71-43-2	0.015	0.001	6
5	n-Butanenitrile	109-74-0	0.018	0.001	3
6	n-Heptane	142-82-5	0.0084	0.0009	10
7	Toluene	108-88-3	0.094	0.002	2
8	n-Octane	111-65-9	0.0094	0.0007	8
9	n-Nonane	111-84-2	0.0042	0.0001	2
10	n-Dodecane	112-40-3	0.0032	0.0003	8
11	n-Tridecane	629-50-5	0.0066	0.0005	8

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples.

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

Table 4-3
Tank S-102 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	1,1-Dichloroethene (vinylidene chloride)	75-35-4	0.0022	0.0003	15
2	Propanenitrile	107-12-0	0.0063	0.0016	25
3	n-Pentanenitrile	110-59-8	0.00080	0.00005	7
4	2-Hexanone	591-78-6	0.0034	0.0007	21
5	n-Hexanenitrile	628-73-9	0.00026	0.00002	9
6	2-Heptanone	110-43-0	0.0024	0.0003	12
7	n-Heptanenitrile	629-08-3	0.00024	0.00005	20
8	2-Octanone	111-13-7	0.00077	0.00016	20
9	n-Decane	124-18-5	0.0027	0.0001	4
10	n-Undecane	1120-21-4	0.0026	0.0001	4

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

² CAS = Chemical Abstract Service.

³ Average of 3, 1-L TST samples.

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

Table 4-4
Tank S-102 Positively Identified Organic Compounds in TST Samples
for which Practical Holding Times were Exceeded --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Butanal ⁵	123-72-8	0.059	0.002	3
2	1-Butanol ⁶	71-36-3	0.39	0.02	5
3	2-Pentanone ⁵	107-87-9	0.0066	0.0003	4

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples.

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

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

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

Table 4-5
Tank S-102 Comparison of Organic Compounds in TST and SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory
and Oak Ridge National Laboratory

Compound	CAS ¹ Number	TST Average ² (ppmv)	SUMMA™ Average ³ (ppmv)	PRD ⁴ (%)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	0.0022	< 0.005	--
Dichloromethane (methylene chloride)	75-09-2	< 0.0053	< 0.005	--
Propanone (acetone)	67-64-1	0.10	0.56	139
Ethanenitrile (acetonitrile)	75-05-8	0.081	0.039	70
Propanenitrile	107-12-0	0.0063	< 0.005	> 23
nButanenitrile	109-74-0	0.018	< 0.005	> 113
Benzene	71-43-2	0.015	0.019	24
Toluene	108-88-3	0.094	0.20	72
n-Hexane	110-54-3	0.0071	< 0.005	> 35
n-Heptane	142-82-5	0.0084	0.012	35
n-Decane	124-18-5	0.0027	< 0.005	--

1 CAS = Chemical Abstract Service.

2 Average of 3, 1-L TST samples by ORNL.

3 Average of 3 samples by PNL.

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

Table 4-6
Tank S-102 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard ³ Deviation (mg/m ³)
1	Propene ⁴	115-07-1	0.43	< 0.35
2	Propane ⁴	74-98-6	0.34	< 0.21
3	Cyclopropane ⁴	75-19-4	0.10	< 0.005
3	Methanol (methyl alcohol)	67-56-1	4.49	0.70
4	1-Butene	106-98-9	0.40	0.06
5	n-Butane	106-97-8	0.24	0.01
6	1-Propene, 2-methyl- ⁴	115-11-7	0.06	< 0.005
7	Ethanol	64-17-5	9.44	0.30
8	2-Propanol ⁵ (isopropyl alcohol)	67-63-0	0.24	--
9	n-Pentane ⁵	109-66-0	0.07	--
10	2-Butanol	78-92-2	0.14	0.02
11	1-Butanol	71-36-3	1.18	0.19
12	N-Nitrosodimethylamine ⁵	62-75-9	0.03	--
13	Pyrazine ⁴	290-37-9	0.05	< 0.01
Sum of tentatively identified compounds:			16.87	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples. Presented values are estimated.

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

4 Detected in only 2 samples.

5 Detected in only 1 sample.

Table 4-7
Tank S-102 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	1-Propene, 2-methyl-	115-11-7	0.047	0.041
2	Methanol (methyl alcohol)	67-56-1	1.55	0.14
3	Ethanol	64-17-5	3.91	0.37
4	Trichlorofluoromethane	75-69-4	0.043	0.074
5	2-Propanol (isopropyl alcohol)	67-63-0	0.16	0.01
6	1-Propanol	71-23-8	0.078	0.009
7	2-Butanol, (R)-	14898-79-4	0.015	0.026
8	Furan, tetrahydro-	109-99-9	0.056	0.010
9	Silane, dimethoxydimethyl-	1112-39-6	0.019	0.033
10	1,4-Dioxane	123-91-1	0.040	0.035
11	1,4-Dioxane and others		0.027	0.046
12	Pyrazine	290-37-9	0.13	0.01
13	Aziridine, 2-methyl-	75-55-8	0.046	0.080
14	N-Nitrosodimethylamine	62-75-9	0.10	0.01
15	Cyclotrisiloxane, hexamethyl-	541-05-9	0.14	0.09
16	1-Propanone, 1-[4-(tri-methylsilyl)oxyphenyl]	33342-89-1	0.013	0.023
17	2-Heptanone, 6-methyl and others		0.010	0.018
18	Cyclotetrasiloxane, octamethyl-	556-67-2	0.066	0.028
19	Alkyl nitrile		0.037	0.005
20	Oxazole, 4,5-dimethyl-2-propyl-	53833-32-2	0.047	0.014
21	Benzyl Alcohol	100-51-6	0.0077	0.0134
22	Benzoic acid, 2-[(trimethylsilyloxy)-trimethylsilyl ester	3789-85-3	0.010	0.018
23	Isopropyl Palmitate	142-91-6	0.054	0.094
24	Benzenesulfonamide, n-butyl-	3622-84-2	0.054	0.011
Sum of tentatively identified compounds:			6.66	

1 CAS = Chemical Abstract Service.

2 Average of 3, 1-L TST samples. Values presented are estimated.

Table 4-8
Tank S-102 Tentatively Identified Organic Compounds in TST Samples
Sorted Alphanumerically --
Analyses by Oak Ridge National Laboratory

Cmp d #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	1-Propene, 2-methyl-	115-11-7	0.047	0.041
16	1-Propanone, 1-[4-(tri-methylsilyl)oxyphenyl]	33342-89-1	0.013	0.023
6	1-Propanol	71-23-8	0.078	0.009
10	1,4-Dioxane	123-91-1	0.040	0.035
11	1,4-Dioxane and others		0.027	0.046
17	2-Heptanone, 6-methyl and others		0.010	0.018
7	2-Butanol, (R)-	14898-79-4	0.015	0.026
5	2-Propanol (isopropyl alcohol)	67-63-0	0.16	0.01
19	Alkyl nitrile		0.037	0.005
13	Aziridine, 2-methyl-	75-55-8	0.046	0.080
24	Benzenesulfonamide, n-butyl-	3622-84-2	0.054	0.011
22	Benzoic acid, 2-[(trimethylsilyloxy]-trimethylsilyl ester	3789-85-3	0.010	0.018
21	Benzyl Alcohol	100-51-6	0.0077	0.0134
18	Cyclotetrasiloxane, octamethyl-	556-67-2	0.066	0.028
15	Cyclotrisiloxane, hexamethyl-	541-05-9	0.14	0.09
3	Ethanol	64-17-5	3.91	0.37
8	Furan, tetrahydro-	109-99-9	0.056	0.010
23	Isopropyl Palmitate	142-91-6	0.054	0.094
2	Methanol (methyl alcohol)	67-56-1	1.55	0.14
14	N-Nitrosodimethylamine	62-75-9	0.10	0.01
20	Oxazole, 4,5-dimethyl-2-propyl-	53833-32-2	0.047	0.014
12	Pyrazine	290-37-9	0.13	0.01
9	Silane, dimethoxydimethyl-	1112-39-6	0.019	0.033
4	Trichlorofluoromethane	75-69-4	0.043	0.074

¹ CAS = Chemical Abstract Service.

² Average of 3, 1-L TST samples. Values presented are estimated.

Table 4-9
Tank S-102 Tentatively Identified Organic Compounds in TST Samples
Sorted by Estimated Concentration --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² e (mg/m ³)	Standard Deviation (mg/m ³)
3	Ethanol	64-17-5	3.91	0.37
2	Methanol (methyl alcohol)	67-56-1	1.55	0.14
5	2-Propanol (isopropyl alcohol)	67-63-0	0.16	0.01
15	Cyclotrisiloxane, hexamethyl-	541-05-9	0.14	0.09
12	Pyrazine	290-37-9	0.13	0.01
14	N-Nitrosodimethylamine	62-75-9	0.10	0.01
6	1-Propanol	71-23-8	0.078	0.009
18	Cyclotetrasiloxane, octamethyl-	556-67-2	0.066	0.028
8	Furan, tetrahydro-	109-99-9	0.056	0.010
24	Benzenesulfonamide, n-butyl-	3622-84-2	0.054	0.011
23	Isopropyl Palmitate	142-91-6	0.054	0.094
1	1-Propene, 2-methyl-	115-11-7	0.047	0.041
20	Oxazole, 4,5-dimethyl-2-propyl-	53833-32-2	0.047	0.014
13	Aziridine, 2-methyl-	75-55-8	0.046	0.080
4	Trichlorofluoromethane	75-69-4	0.043	0.074
10	1,4-Dioxane	123-91-1	0.040	0.035
19	Alkyl nitrile		0.037	0.005
11	1,4-Dioxane and others		0.027	0.046
9	Silane, dimethoxydimethyl-	1112-39-6	0.019	0.033
7	2-Butanol, (R)-	14898-79-4	0.015	0.026
16	1-Propanone, 1-[4-(tri-methylsilyl)oxyphenyl]	33342-89-1	0.013	0.023
22	Benzoic acid, 2-[(trimethylsilyloxy)-trimethylsilyl ester	3789-85-3	0.010	0.018
17	2-Heptanone, 6-methyl and others		0.010	0.018
21	Benzyl Alcohol	100-51-6	0.0077	0.0134

¹ CAS = Chemical Abstract Service.

² Average of 3, 1-L TST samples. Values presented are estimated.

WHC-SD-WM-ER-446 REV. 1