Accession #: D196054848

Document #: SD-WM-ER-460

Title/Desc:

TANK 241SX106 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
3/1995

[illegible]

COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 2

1. ECN 626288

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 [X] No	4. Date 09/27/95
	5. Project Title/No./Work Order No. TANK 241-SX-106 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-460 REV X0	9. Related ECN No(s). N/A	10. Related PO No. N/A

11a. Modification Work [] Yes (fill out Blk. 11b) [X] 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	[X]	Design Improvement	[]	Environmental	[]	Facility Deactivation	[]
As-Found	[]	Facilitate Const	[]	Const. Error/Omission	[]	Design Error/Omission	[]

13b. Justification Details

Complete rewrite which includes all vapor sampling events to date and data qualification.

14. Distribution (include name, MSIN, and no. of copies)

See attached Distribution Sheet

RELEASE STAMP

OFFICIAL RELEASE
BY WHC
DATE SEP 26 1995
Sta. 4

3

ENGINEERING CHANGE NOTICE

Page 2 of 2

1. ECN (use no. from pg. 1)
626288

15. Design Verification Required
☐ Yes
☒ No

16. Cost Impact

ENGINEERING		CONSTRUCTION	
Additional	☐ $	Additional	☐ $
Savings	☐ $	Savings	☐ $

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

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
OPERATIONS AND ENGINEERING		
Cog. Eng.	D. R. Bratzel DRB	9/25/95
Cog. Mgr.	T. J. Kelley	9/25/95
QA		
Safety		
Environ.		
Other		
Proj.		
Proj.		
Proj.		
Proj.		

	Signature	Date
ARCHITECT-ENGINEER		
PE		
QA		
Safety		
Design		
Environ.		
Other		
DEPARTMENT OF ENERGY		
Signature or a Control Number that tracks the Approval Signature		
ADDITIONAL		

RELEASE AUTHORIZATION

Document Number: WHC-SD-WM-ER-460, REV 1

Document Title: Tank 241-SX-106 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

Kara Broz

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

THIS PAGE INTENTIONALLY LEFT BLANK

SUPPORTING DOCUMENT

1. Total Pages 34

2. Title

TANK 241-SX-106 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN MARCH 1995

3. Number

WHC-SD-WM-ER-460

4. Rev No.

1

5. Key Words

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

6. Author

Name: D. R. BRATZEL

DRBratzel 9/25/95

Signature

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
BY WHC
DATE SEP 26 1995

THIS PAGE INTENTIONALLY
LEFT BLANK

RECORD OF REVISION	(1) Document Number WHC-SD-WM-ER-460	Page 1

(2) Title

TANK 241-SX-106 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN MARCH 1995

CHANGE CONTROL RECORD

(3) Revision	(4) Description of Change - Replace, Add, and Delete Pages	Authorized for Release (5) Cog. Engr.	 (6) Cog. Mgr. Date
0	(7) WHC-SD-WM-ER-460, REV. 0, EDT 612347 May 31, 1995		
1 RS	Complete revision and title change. ECN 626288	DEB	9/25/95

WHC-SD-WM-ER-460
Revision 1
UC-2070

Tank 241-SX-106 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

THIS PAGE INTENTIONALLY
LEFT BLANK

WHC-SD-WM-ER-460 REV. 1

Tank 241-SX-106 Headspace Gas and Vapor Characterization Results for Samples Collected in March 1995

September 19, 1995

J. L. Huckaby
Multimedia Exposure Assessment
Pacific Northwest Laboratories

D. R. Bratzel
Waste Tank Characterization Program
Westinghouse Hanford Company

THIS PAGE INTENTIONALLY
LEFT BLANK

Contents

1.0 INTRODUCTION 1
  1.1 Characterization Objectives 1
  1.2 Characterization Data Criteria 1
  1.3 Sampling Overview 2
  1.3 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 4
  3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium 5
  3.4 Discussion of Inorganic Gases and Vapors 5

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-SX-106 Headspace Gas and Vapor Characterization Results

for Samples Collected in March 1995

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank SX-106 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 SX-106 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

1.2 Characterization Data Criteria

Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution describes parameters for data collection to ensure appropriate conclusions can be drawn from the data. Tank headspace characterization data were collected to help in the evaluation of 1) headspace flammability, and 2) identification and quantification of compounds of toxicological concern.

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). However, current governing operating specifications for single shell Watchlist waste tanks, such as tank SX-106, 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 headspace characterization data presented here are from a single sampling event. Samples collected are thought to have been reasonably representative of the tank SX-106 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). However, tank SX-106 is an actively ventilated tank, and the representativeness of the samples depends on such parameters as ventilation flow rate and locations of all air inlets and outlets as well as the sample collection point. A prime consideration is the ventilation rate, which is not well known. Furthermore, no assessment has been made of how the tank SX-106 ventilation rate or headspace composition changes with time.

1.3 Tank Headspace Dynamics

Tank SX-106 is the third tank in a 3-tank cascade with tanks SX-104 and SX-105. Tanks SX-104 and SX-105 are connected via underground piping, and similar piping connects tanks SX-105 and SX-106. By design, the ventilation of tanks SX-104 and SX-105 occurs via the underground piping and through tank SX-103. Since the piping connects the headspaces of these tanks, gases and vapors originating from the wastes in tanks SX-104 and SX-105 are transferred to tank SX-106. At this time, however, no headspace characterization data is available for either tanks SX-102 or SX-101 to assess their potential effect on tank SX-106.

Unlike most passively ventilated tanks, for which characterization of the headspace provides direct evidence of volatile constituents of the waste, the active ventilation of tank SX-103 and the fact that other tanks are vented through it negates direct use of the data for that purpose. The headspace characterization data is still presumed to be the best available for assessing flammability and industrial hygiene concerns.

2.0 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank SX-106 using the vapor sampling system (VSS) on March 24, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-SX-106 Tank Characterization Plan* (Homi 1995a). The tank headspace temperature was determined to be 30 °C. Air from the tank SX-106 headspace was withdrawn from a single elevation via a 6.7-m long heated sampling probe mounted in riser 14, 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 9:24 a.m. and 1:00 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™[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 SUMMA™ canisters were prepared and analyzed by PNL at PNL quality assurance impact level 2 (Klinger et al. 1995). PNL analyses of SUMMA™ canisters and sorbent traps for inorganic compounds were performed 11 and 13 days respectively after sample collection (Ligotke 1995). Both SUMMA™ canister, and sorbent trap analyses were within the maximum 60-day holding time allowed by the WHC quality assurance project plan (Keller 1994).

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Ammonia concentration in headspace of tank SX-106 was measured as 179 ppmv. Ammonia has been observed in virtually all of the passively ventilated waste tanks sampled to date, at concentrations ranging from about 3 ppmv in tank C-108 (Lucke et al. 1995), to 1040 ppmv in BY-108 (McVeety et al. 1995). However, the measured concentration of ammonia in tank SX-106 can not be easily compared to that of the passively ventilated tanks, because its ventilation rate is not well known, and the rate at which it receives ammonia vapor from tanks SX-104 and SX-105 is likewise unknown, Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 179 ppmv corresponds to about 0.12 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank SX-106 was determined to be < 98 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, a 98 ppmv hydrogen concentration in tank SX-106 would correspond to about 0.24 % of its LFL. At this level, hydrogen is not a flammability concern in tank SX-106.

The reported nitrous oxide concentration, 14 ppmv, is very near the analytical method detection limit, and in 2 of the 3 SUMMA™ samples, nitrous oxide was measured to be < 12.6 ppmv. 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 SX-106 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide concentration in the tank SX-106 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 in the passively ventilated tanks, 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-103[2] (Huckaby and Story 1994).

---

[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 placed in brackets to emphasize it should be considered secondary data.

The carbon dioxide concentration in the tank SX-106 headspace, measured at an average 107 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 SX-106 gas and vapor sampling event, for example, were measured to have an average 359 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. The 107 ppmv of carbon dioxide in the tank SX-106 headspace is typical of values for the passively ventilated waste tanks sampled to date.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank SX-106 headspace were both determined to be ≤ 0.02 ppmv. These are acid gases that would have very low equilibrium concentrations above the high pH sludge in tank SX-106. 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 SX-106 headspace.

The water vapor concentration of tank SX-106 was determined to be about 14.9 mg/L, at the measured tank headspace temperature of 30 °C and pressure of 990 mbar (742.3 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 19.9 mbar (14.9 torr), to a dew point of 17.5 °C, and to a relative humidity of 47 %.

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

3.4 Discussion of Inorganic Gases and Vapors

Aside from water vapor, the most abundant waste constituents in the tank SX-106 headspace are ammonia and nitrous oxide. These have been detected in most tank headspaces sampled to date and, along with hydrogen, are usually the dominate waste species. The concentration of ammonia is relatively high given that tank SX-106 is actively ventilated.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are good for the methods used. Relative standard deviations range from less than 1 % for water vapor to about 3 % for ammonia and carbon dioxide results. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), small relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

4.0 ORGANIC VAPORS

Organic vapors in the tank SX-106 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Both PNL and ORNL used a gas chromatograph (GC) equipped with a mass spectrometer (MS) detector to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Klinger et al. (1995).

SUMMA™ sample results should be considered the primary organic vapor data for tank SX-106. PNL results were produced at PNL quality assurance impact level 2. All PNL organic vapor analyses were completed 19 days after sample collection, and were within the maximum 60-day holding time (Keller 1994). However, the 60-day holding time was administratively chosen, and 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 tank C-103.

Table 4-1 lists 4 organic compounds positively identified and quantitated in SUMMA™ samples, and the measured methane concentration. SUMMA™ analyses of organic compounds were performed according to the TO-14 methodology, except for the analysis of methane, which was analyzed with the inorganic gases (Klinger et al. 1995). None of the 39 TO-14 target analytes and only 4 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 20 of 27 target analytes in TST samples. Dichloromethane, n-pentanenitrile, octane, n-hexanenitrile, n-heptanenitrile, dibutyl butylphosphonate, and tributyl phosphate were the only TST target analytes not detected. Tables 4-2, 4-3, and 4-4 list the compounds that were positively identified in 4 TST samples, with their average concentrations. Table 4-2 lists 3 compounds which were quantitatively measured, Table 4-3 lists 15 compounds which were not quantitatively measured because the measured value in at least 1 TST sample was outside the instrument calibration range, and Table 4-4 lists the 2 compounds which exceeded their analyte-specific ORNL practical holding times. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so that no analyte appears in more than 1 of these tables. Data in Tables 4-3 and 4-4 may not be accurate to within ± 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 and 1-butanol exceeded their practical holding times, and may have been affected by the 32 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, and 1--butanol as 1, and 17 days respectively. It should be noted that the contractual holding time for the TST samples was 60 days.

There were 11 target analytes 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 fairly good agreement. As indicated in Table 4-5, the reported concentrations of 1,1-dichloroethene and ethanenitrile in TST samples are higher than in SUMMA™ samples, and the reported concentration of propanone is higher in SUMMA™ samples than in TST samples. The target analytes are generally only present at very low concentrations.

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 SX-106 and obtain concentration in ppmv of analyte in moist tank air, multiply the dry-air ppmv concentrations by 0.980.

The only analyte in Tables 4-1 through 4-4 above 0.1 ppmv is 1-butanol, measured to be about 0.13 ppmv in TST samples. 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 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. Only non-zero results are included in the reported averages. The tentatively identified compounds detected in TST samples, and their estimated concentrations, are listed in Table 4-7. Compounds are listed in Table 4-7 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table 4-7 are all 4-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Estimated concentrations are in mg/m^3, based on dry air at 0 °C and 1.01 bar.

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

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and Klinger et al. (1995), respectively, and should be reviewed before this data are used for decision making. Concentrations given in Tables 4-6 through 4-9 should be considered rough estimates.

4.3 Discussion of Organic Compounds

The organic compounds listed in Tables 4-1 through 4-9 may be classified as either 1) organic compounds added to tank SX-106 as waste that are still evaporating, or 2) organic compounds that have been generated by reactions of the original waste.

The first class 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, and n-tetradecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs). Though NPHs are positively identified in tank SX-106, 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 # 24, and the split peak of Cmpd # 39 and 40 in Table 4-7), and other silicon-containing compounds (e.g., Cmpd # 10 and 14 in Table 4-7) may also have been sent to tank SX-106 with other wastes. Small quantities of organo-silicon compounds may have been introduced to the waste tank through their use as defoaming agents, and they may also be present in the headspace due to their use in liquid traps at the tank's breather riser. Several of these have been observed in TST blanks, however, and they may be present as artifacts of the gas chromatography process. Chlorotrimethylsilane (Cmpd # 5 in Table 4-7) reacts very rapidly with water, and it is not reasonable to think it actually exists in the SX-106 headspace.

The absence of tributyl phosphate in the tank SX-106 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 SX-106 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 SX-106 headspace samples should not be taken as proof it is not present in the headspace or the waste.

The second class 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, ketones, nitriles, alkenes, and volatile alkanes, all of which have been associated with the degradation of the NPHs.

On the basis of mass concentration, alcohols are the dominate type of organic compound in the tank SX-106 headspace. Methanol, ethanol, 1-propanol, and 1-butanol account for 92 % of the total estimated concentration of organic compounds in SUMMA™ samples. 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 SX-106 has relatively few nitrile or ketones, and no aldehydes were detected.

A relatively large number of nitrogen-containing cyclic compounds were also detected in TST samples from tank SX-106, including pyridines, pyrazines, pyrroles, an oxazole, a piperidine, and an indole. Because the overall level of organic vapors is low, and relatively large TST sample volumes were collected, these compounds were detectible in the tank SX-106 TST samples. These compounds may be present at similar levels in other waste tanks, but because larger quantities of other organic vapors are usually present, their presence may be obscured.

The total organic vapor concentration of tank SX-106 was estimated by Jenkins et al. (1995a) to be about 1.5 mg/m^3 from the analysis of 4 TST samples by GC/MS. A similar summation of organic compounds measured in SUMMA™ samples from tank SX-106 provides an estimated total organic vapor concentration of 2.4 mg/m^3. This disagreement is largely due to the different estimated concentrations of the volatile alcohols in the 2 sample types. Volatile alcohols may not be quantitatively recovered from TST samples.

The organic vapor concentrations in tank SX-106 are low compared to the passively ventilated waste tanks that have been sampled. The organic vapors in tank SX-106 clearly indicate the presence of the semivolatile NPHs and their degradation products in the tank headspace, though the NPHs are at trace levels. Tributyl phosphate was not detected in any of the headspace samples, but there is circumstantial evidence that it is also present.

Tank SX-106 is the only 241-SX 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, as well as tank S-102 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 SX-106 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 specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995b). However, the measured ammonia concentration of 179 ppmv does exceed the industrial hygiene notification limit of 150 ppmv.

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-SX-106 Tank Characterization Plan*, WHC-SD-WM-TP-314 Rev. 0, 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., H. Babad, and D. R. Bratzel, 1995, *Headspace Gas and Vapor Characterization Summary for the 43 Vapor Program Suspect Tanks*, WHC-SD-WM-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 090195 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-SX-106 Headspace Components*, ORNL-CASD-FR-241SX106.95 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. Ligotke, K. H. Pool, R. B. Lucke, B. D. McVeety, K. B. Olsen, O. P. Bredt, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-SX-106: Results from Samples Collected on 3/24/95*, PNL-10584 UC-606, Pacific Northwest Laboratory, Richland, Washington.

Ligotke, M. W., 1995, *PNL Vapor Project Analytical Holding Times*, (Letter to D.R. Bratzel, September 23, 1995), Pacific Northwest Laboratories, Richland, Washington.

Lucke, R. B., M. W. Ligotke, 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. Ligotke, 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.

Meachem, J.E., H. Babad, R.J. Cash, G.T. Dukelow, S.J. Eberlein, D.W. Hamilton, G.D. Johnson, J.W. Osborne, M.A. Payne, D.J. Sherwood, D.A. Turner, and J.L. Huckaby, 1995, *Approach for Tank Safety Characterization of Hanford Site Waste*, WHC-WP-0843 Rev.0, UC-2070, Westinghouse Hanford Company, 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.

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-SX-106 Using the Vapor Sampling System*, WHC-SD-WM-RPT-145 Rev. 0, Westinghouse Hanford Company, Richland, Washington.

Table 2-1
Tank SX-106 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 SX-106 Inorganic Gas and Vapor Concentrations -- Analyses Conducted 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	179	5	3
Carbon Dioxide, CO_2	124-38-9	SUMMA™	3	107	3	3
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 12	--	--
Hydrogen, H_2	1333-74-0	SUMMA™	3	< 98	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.02	--	--
Nitrogen Dioxide, NO_2	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide[3], N_2O	10024-97-2	SUMMA™	3	14	--	--
Water Vapor, H_2O	7732-18-5	Sorbent Trap	6	20,100 (14.9 mg/L)	90 (0.07 mg/L)	0.5

1 CAS = Chemical Abstracts Service.

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

3 Detected in only 1 sample.

Table 4-1
Tank SX-106 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	Propanone (acetone)	67-64-1	0.021	0.001	6
2	1-Propanol	71-23-8	0.041	0.036	87
3	Tetrahydrofuran	109-99-9	0.007	0.0003	4
4	Pyridine	110-86-1	0.015	0.012	81
5	Methane	74-82-8	< 12	--	--
Sum of positively identified compounds:			0.23	mg/m³	

[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 SX-106 Quantitatively Measured Organic Compounds in TST Samples -- Analyses by Oak Ridge National Laboratory[1]

Cmpd #	Compound	CAS[2] Number	Average[3] (ppmv)	Standard Deviation (ppmv)	RSD[4] (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.018	0.001	6
2	Propanone (acetone)	67-64-1	0.012	0.002	20
3	1,1-Dichloroethene (vinylidene chloride)	75-35-4	0.0050	0.0036	72

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

2 CAS = Chemical Abstract Service.

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

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

Table 4-3
Tank SX-106 Positively Identified Organic Compounds in TST Samples -- Analyses by Oak Ridge National Laboratory[1]

Cmpd #	Compound	CAS[2] Number	Average[3] (ppmv)	Standard Deviation (ppmv)	RSD[4] (%)
1	Propanenitrile	107-12-0	0.0010	0.0001	10
2	n-Hexane	110-54-3	0.00070	0.00031	44
3	Benzene	71-43-2	0.00055	0.00014	25
4	n-Butanenitrile	109-74-0	0.0032	0.0003	10
5	2-Pentanone	107-87-9	0.00040	0.00015	36
6	n-Heptane	142-82-5	0.00025	0.00005	20
7	Toluene	108-88-3	0.00055	0.00015	28
8	2-Hexanone	591-78-6	0.00026	0.00009	34
9	2-Heptanone	110-43-0	0.00032	0.00013	39
10	n-Nonane	111-84-2	0.00020	0.00006	31
11	2-Octanone	111-13-7	0.00018	0.00008	43
12	n-Decane	124-18-5	0.00019	0.00006	34
13	n-Undecane	1120-21-4	0.00052	0.00008	16
14	n-Dodecane	112-40-3	0.00045	0.00011	24
15	n-Tridecane	629-50-5	0.00062	0.00015	25

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

2 CAS = Chemical Abstract Service.

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

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

Table 4-4
Tank SX-106 Positively Identified Organic Compounds in TST Samples for which Practical Holding Times were Exceeded -- Analyses by Oak Ridge National Laboratory[1]

Cmpd #	Compound	CAS[2] Number	Average[3] (ppmv)	Standard Deviation (ppmv)	RSD[4] (%)
1	Butanal[5]	123-72-8	0.022	0.002	7
2	1-Butanol[6]	71-36-3	0.13	0.01	7

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

2 CAS = Chemical Abstract Service.

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

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

5 The concentration of this analyte 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 SX-106 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	0.0050	< 0.005	0
Dichloromethane (methylene chloride)	75-09-2	< 0.0013	< 0.005	--
Propanone (acetone)	67-64-1	0.012	0.021	54
Ethanenitrile (acetonitrile)	75-05-8	0.018	< 0.005	> 113
Propanenitrile	107-12-0	0.0010	< 0.005	--
n-Butanenitrile	109-74-0	0.0032	< 0.005	--
Benzene	71-43-2	0.00055	< 0.005	--
Toluene	108-88-3	0.00055	< 0.005	--
n-Hexane	110-54-3	0.00070	< 0.005	--
n-Heptane	142-82-5	0.00025	< 0.005	--
n-Decane	124-18-5	0.00019	< 0.005	--

1 CAS = Chemical Abstract Service.

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

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 SX-106 Tentatively Identified Organic Compounds in SUMMA™ Samples -- Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
1	Methanol (methyl alcohol)	67-56-1	1.34	0.05
2	Ethanol	64-17-5	0.38	0.01
3	1-Butanol	71-36-3	0.41	0.01
Sum of tentatively identified compounds:			2.13	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples, values presented are estimated.

Table 4-7
Tank SX-106 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	0.00074	0.00148
2	Methanol (methyl alcohol)	67-56-1	0.18	0.03
3	Ethanol	64-17-5	0.084	0.012
4	Trichlorofluoromethane	75-69-4	0.0088	0.0051
5	Silane, chlorotrimethyl-	75-77-4	0.0054	0.0109
6	2-Propanol (isopropyl alcohol)	67-63-0	0.014	0.004
7	2,3-Dimethyl-1, 4-pentadiene	758-86-1	0.0019	0.0038
8	1-Propanol	71-23-8	0.011	0.007
9	Benzeneacetic acid, .alpha.-hydroxy ethyl ester	774-40-3	0.0034	0.0068
10	Silanol, trimethyl-	1066-40-6	0.0053	0.0106
11	Mixture		0.0021	0.0042
12	Ester of Acetic Acid		0.0017	0.0034
13	Furan, tetrahydro-	109-99-9	0.0076	0.0055
14	Silane, dimethoxydimethyl-	1112-39-6	0.012	0.012
15	1,4-Dioxane	123-91-1	0.0096	0.0003
16	Mixture		0.0017	0.0033
17	Pyrazine	290-37-9	0.014	0.001
18	Propane, 2-methyl-2-nitro-	594-70-7	0.0039	0.0026
19	N-Nitrosodimethylamine	62-75-9	0.025	0.010
20	1-ethyl-6-ethylidene cyclohexene	61141-57-9	0.0037	0.0073
21	(S)-(+)-1,2-Propanediol	4254-15-3	0.12	0.20
22	Phenol,4-(aminomethyl)-2-methoxy	'1196-92-5	0.0053	0.0106
23	Benzothiazole, 2-phenyl-	883-93-2	0.016	0.031
24	Cyclotrisiloxane, hexamethyl-	541-05-9	0.15	0.25
25	Pyrazine, methyl-	109-08-0	0.00059	0.00117
26	Oxazole, 4,5-dihydro-2-methyl-	1120-64-5	0.0061	0.0041

Cmpd #	Compounds	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
27	1H-Pyrrole, 2,5-dimethyl-	625-84-3	0.0029	0.0057
28	Benzene, 1,3-dimethyl- and others		0.0017	0.0019
29	2-Propen-1-ol	107-18-6	0.0071	0.0049
30	3-Heptanone	106-35-4	0.00080	0.00160
31	Ethanol, 2-butoxy- and others		0.0015	0.0018
32	Pyrazine, ethyl-	13925-00-3	0.00075	0.00150
33	Pyrazine, ethyl- and butyrolactone		0.0010	0.0020
34	1-Pentyn-3-ol, 3,4-dimethyl-	1482-15-1	0.00069	0.00137
35	9-Decen-2-one and others		0.00081	0.00163
36	6-Amino-2,3-diphenyl(1H) pyrrolo[2,3-b]pyridine		0.0040	0.0080
37	Benz[a]acridine, 8,10-diethyl and others		0.00073	0.00147
38	2-Buten-1-ol, (Z)-	4088-60-2	0.0039	0.0030
39	Cyclotetrasiloxane, octamethyl-	556-67-2	0.055	0.082
40	Cyclotetrasiloxane, octamethyl-	556-67-2	0.0023	0.0046
41	1-Hexanol, 2-ethyl-	104-76-7	0.0081	0.0012
42	Benzyl Alcohol	100-51-6	0.0066	0.0045
43	2(3H)-Furanone, 5-ethenyl-dihydro-5-methyl-	1073-11-6	0.00062	0.00124
44	Cyclopentane, 2-ethyl-1,1-dimethyl-	54549-80-3	0.00054	0.00109
45	Benzenemethanol, 4-(1,1-dimethylethyl)-a-methyl- and others		0.0061	0.0121
46	Mixture		0.00058	0.00116
47	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.015	0.022
48	Octanamide, N-(2-hydroxyethyl)-	7112-02-9	0.0049	0.0033
49	n-Methyl-3-Piperidine carboxamide	5115-98-0	0.0070	0.0050
50	1H-Indole, 2-phenyl-	948-65-2	0.0014	0.0028
51	2-Hexenedioic acid, bis (trimethylsilyl) ester	55494-10-5	0.0023	0.0046
52	Tetradecane	629-59-4	0.0028	0.0023

Cmpd #	Compounds	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
53	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	0.0040	0.0029
54	Mixture		0.0040	0.0047
55	2-Propen-1-one, 3-(2-furanyl)-1-phenyl-	717-21-5	0.0013	0.0026
56	Benzenesulfonamide, n-butyl	3622-84-2	0.055	0.035
57	1-Pentadecene	13360-61-7	0.00098	0.00196
58	Nonadecane	629-92-5	0.00064	0.00129
59	Hexadecanoic acid	57-10-3	0.0063	0.0126
60	Isopropyl Palmitate	142-91-6	0.0028	0.0032
Sum of tentatively identified compounds:			0.91	

[1] CAS = Chemical Abstract Service.

[2] Average of 4 samples; 3 were 4-L and 1 was 1-L, presented values are estimated.

Table 4-8
Tank SX-106 Tentatively Identified Organic Compounds in TST Samples Sorted Alphanumerically -- Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
21	(S)-(+)-1,2-Propanediol	4254-15-3	0.12	0.20
1	1-Propene, 2-methyl-	115-11-7	0.00074	0.00148
34	1-Pentyn-3-ol, 3,4-dimethyl-	1482-15-1	0.00069	0.00137
57	1-Pentadecene	13360-61-7	0.00098	0.00196
8	1-Propanol	71-23-8	0.011	0.007
20	1-ethyl-6-ethylidene-cyclohexene	61141-57-9	0.0037	0.0073
41	1-Hexanol, 2-ethyl-	104-76-7	0.0081	0.0012
15	1,4-Dioxane	123-91-1	0.0096	0.0003
27	1H-Pyrrole, 2,5-dimethyl-	625-84-3	0.0029	0.0057
50	1H-Indole, 2-phenyl-	948-65-2	0.0014	0.0028
51	2-Hexenedioic acid, bis (trimethylsilyl) ester	55494-10-5	0.0023	0.0046
55	2-Propen-1-one, 3-(2-furanyl)-1-phenyl-	717-21-5	0.0013	0.0026
38	2-Buten-1-ol, (Z)-	4088-60-2	0.0039	0.0030
29	2-Propen-1-ol	107-18-6	0.0071	0.0049
7	2,3-Dimethyl-1, 4-pentadiene	758-86-1	0.0019	0.0038
43	2(3H)-Furanone, 5-ethenyl-dihydro-5-methyl-	1073-11-6	0.00062	0.00124
6	2-Propanol (isopropyl alcohol)	67-63-0	0.014	0.004
30	3-Heptanone	106-35-4	0.00080	0.00160
36	6-Amino-2,3-diphenyl(1H) pyrrolo[2,3-b]pyridine		0.0040	0.0080
35	9-Decen-2-one and others		0.00081	0.00163
28	Benzene, 1,3-dimethyl- and others		0.0017	0.0019
9	Benzeneacetic acid, .alpha.-hydroxy ethyl ester	774-40-3	0.0034	0.0068

Cmpd #	Compounds	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
45	Benzenemethanol, 4-(1,1-dimethylethyl)-a-methyl- and others		0.0061	0.0121
56	Benzenesulfonamide, n-butyl-	3622-84-2	0.055	0.035
47	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.015	0.022
23	Benzothiazole, 2-phenyl-	883-93-2	0.016	0.031
42	Benzyl Alcohol	100-51-6	0.0066	0.0045
37	Benz[a]acridine, 8,10-diethyl- and others		0.00073	0.00147
44	Cyclopentane, 2-ethyl-1,1-dimethyl-	54549-80-3	0.00054	0.00109
39	Cyclotetrasiloxane, octamethyl-	556-67-2	0.055	0.082
40	Cyclotetrasiloxane, octamethyl-	556-67-2	0.0023	0.0046
24	Cyclotrisiloxane, hexamethyl-	541-05-9	0.15	0.25
12	Ester of Acetic Acid		0.0017	0.0034
3	Ethanol	64-17-5	0.084	0.012
31	Ethanol, 2-butoxy- and others		0.0015	0.0018
13	Furan, tetrahydro-	109-99-9	0.0076	0.0055
59	Hexadecanoic acid	57-10-3	0.0063	0.0126
60	Isopropyl Palmitate	142-91-6	0.0028	0.0032
2	Methanol (methyl alcohol)	67-56-1	0.18	0.03
11	Mixture		0.0021	0.0042
16	Mixture		0.0017	0.0033
46	Mixture		0.00058	0.00116
54	Mixture		0.0040	0.0047
49	n-Methyl-3-Piperidine carboxamide	5115-98-0	0.0070	0.0050
19	N-Nitrosodimethylamine	62-75-9	0.025	0.010
58	Nonadecane	629-92-5	0.00064	0.00129
48	Octanamide, N-(2-hydroxyethyl)-	7112-02-9	0.0049	0.0033
26	Oxazole, 4,5-dihydro-2-methyl-	1120-64-5	0.0061	0.0041
22	Phenol,4-(aminomethyl)-2-methoxy-	1196-92-5	0.0053	0.0106
18	Propane, 2-methyl-2-nitro-	594-70-7	0.0039	0.0026

Cmpd #	Compounds	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
53	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	0.0040	0.0029
17	Pyrazine	290-37-9	0.014	0.001
25	Pyrazine, methyl-	109-08-0	0.00059	0.00117
32	Pyrazine, ethyl-	13925-00-3	0.00075	0.00150
33	Pyrazine, ethyl- and butyrolactone		0.0010	0.0020
5	Silane, chlorotrimethyl-	75-77-4	0.0054	0.0109
14	Silane, dimethoxydimethyl-	1112-39-6	0.012	0.012
10	Silanol, trimethyl-	1066-40-6	0.0053	0.0106
52	Tetradecane	629-59-4	0.0028	0.0023
4	Trichlorofluoromethane	75-69-4	0.0088	0.0051
Sum of tentatively identified compounds:			0.91	

[1] CAS = Chemical Abstract Service.

[2] Average of 4 samples; 3 were 4-L and 1 was 1-L, presented values are estimated.

Table 4-9
Tank SX-106 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)
2	Methanol (methyl alcohol)	67-56-1	0.18	0.03
24	Cyclotrisiloxane, hexamethyl-	541-05-9	0.15	0.25
21	(S)-(+)-1,2-Propanediol	4254-15-3	0.12	0.20
3	Ethanol	64-17-5	0.084	0.012
39	Cyclotetrasiloxane, octamethyl-	556-67-2	0.055	0.082
56	Benzenesulfonamide, n-butyl-	3622-84-2	0.055	0.035
19	N-Nitrosodimethylamine	62-75-9	0.025	0.010
23	Benzothiazole, 2-phenyl-	883-93-2	0.016	0.031
47	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.015	0.022
6	2-Propanol (isopropyl alcohol)	67-63-0	0.014	0.004
17	Pyrazine	290-37-9	0.014	0.001
45	Benzenemethanol, 4-(1,1-dimethylethyl)- a-methyl- and others		0.0061	0.0121
14	Silane, dimethoxydimethyl-	1112-39-6	0.012	0.012
8	1-Propanol	71-23-8	0.011	0.007
15	1,4-Dioxane	123-91-1	0.0096	0.0003
4	Trichlorofluoromethane	75-69-4	0.0088	0.0051
41	1-Hexanol, 2-ethyl-	104-76-7	0.0081	0.0012
13	Furan, tetrahydro-	109-99-9	0.0076	0.0055
29	2-Propen-1-ol	107-18-6	0.0071	0.0049
49	n-Methyl-3-Piperidine carboxamide	5115-98-0	0.0070	0.0050
42	Benzyl Alcohol	100-51-6	0.0066	0.0045
59	Hexadecanoic acid	57-10-3	0.0063	0.0126
26	Oxazole, 4,5-dihydro-2-methyl-	1120-64-5	0.0061	0.0041
5	Silane, chlorotrimethyl-	75-77-4	0.0054	0.0109

Cmpd #	Compounds	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
10	Silanol, trimethyl-	1066-40-6	0.0053	0.0106
22	Phenol,4-(aminomethyl)-2-methoxy-	1196-92-5	0.0053	0.0106
48	Octanamide, N-(2-hydroxyethyl)-	7112-02-9	0.0049	0.0033
54	Mixture		0.0040	0.0047
36	6-Amino-2,3-diphenyl(1H) pyrrolo[2,3-b]pyridine		0.0040	0.0080
53	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	0.0040	0.0029
18	Propane, 2-methyl-2-nitro-	594-70-7	0.0039	0.0026
38	2-Buten-1-ol, (Z)-	4088-60-2	0.0039	0.0030
20	1-ethyl-6-ethylidene-cyclohexene	61141-57-9	0.0037	0.0073
9	Benzeneacetic acid, .alpha.-hydroxy ethyl ester	774-40-3	0.0034	0.0068
27	1H-Pyrrole, 2,5-dimethyl-	625-84-3	0.0029	0.0057
52	Tetradecane	629-59-4	0.0028	0.0023
60	Isopropyl Palmitate	142-91-6	0.0028	0.0032
51	2-Hexenedioic acid, bis (trimethylsilyl) ester	55494-10-5	0.0023	0.0046
40	Cyclotetrasiloxane, octamethyl-	556-67-2	0.0023	0.0046
11	Mixture		0.0021	0.0042
7	2,3-Dimethyl-1, 4-pentadiene	758-86-1	0.0019	0.0038
28	Benzene, 1,3-dimethyl- and others		0.0017	0.0019
12	Ester of Acetic Acid		0.0017	0.0034
16	Mixture		0.0017	0.0033
31	Ethanol, 2-butoxy- and others		0.0015	0.0018
50	1H-Indole, 2-phenyl-	948-65-2	0.0014	0.0028
55	2-Propen-1-one, 3-(2-furanyl)-1-phenyl-	717-21-5	0.0013	0.0026

Cmpd #	Compounds	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
33	Pyrazine, ethyl- and butyrolactone		0.0010	0.0020
57	1-Pentadecene	13360-61-7	0.00098	0.00196
35	9-Decen-2-one and others		0.00081	0.00163
30	3-Heptanone	106-35-4	0.00080	0.00160
37	Benz[a]acridine, 8,10-diethyl- and others		0.00073	0.00147
32	Pyrazine, ethyl-	13925-00-3	0.00075	0.00150
1	1-Propene, 2-methyl-	115-11-7	0.00074	0.00148
34	1-Pentyn-3-ol, 3,4-dimethyl-	1482-15-1	0.00069	0.00137
58	Nonadecane	629-92-5	0.00064	0.00129
43	2(3H)-Furanone, 5-ethenyl- dihydro-5-methyl-	1073-11-6	0.00062	0.00124
44	Cyclopentane, 2-ethyl-1,1-dimethyl-	54549-80-3	0.00054	0.00109
46	Mixture		0.00058	0.00116
25	Pyrazine, methyl-	109-08-0	0.00059	0.00117
Sum of tentatively identified compounds:			0.91	

1 CAS = Chemical Abstract Service.

2 Average of 4 samples; 3 were 4-L and 1 was 1-L, presented values are estimated.

THIS PAGE INTENTIONALLY
LEFT BLANK