COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 2

1. ECN No 625437

Proj. ECN

2. ECN Category (mark one)	3. Originator's Name, Organization, MSIN, and Telephone No.	3a. USQ Required?	4. Date
Supplemental [ ] Direct Revision [X] Change ECN [ ] Temporary [ ] Standby [ ] Supersedure [ ] Cancel/Void [ ]	D. R. BRATZEL, 75640, S7-21, 373-3579	[ ] Yes [X] No	09/27/95
	5. Project Title/No./Work Order No. TANK 241-BY-103 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN MAY 1994 AND NOVEMBER 1994	6. Bldg./Sys./Fac. No. 2704HV/200E	7. Approval Designator N/A
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11a. Modification Work	11b. Work Package No.	11c. Modification Work Complete	11d. Restored to Original Condition (Temp. or Standby ECN only)
[ ] Yes (fill out Blk. 11b) [X] No (NA Blks. 11b, 11c, 11d)	N/A	N/A Cog. Engineer Signature & Date	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 28 1995

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ENGINEERING CHANGE NOTICE

1. ECN (use no. from pg. 1) 625437

15. Design Verification Required	16. Cost Impact				17. Schedule Impact (days)	
	ENGINEERING		CONSTRUCTION			
[] Yes	Additional	[] $	Additional	[] $	Improvement	[]
[X] No	Savings	[] $	Savings	[] $	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
OPERATIONS AND ENGINEERING		ARCHITECT-ENGINEER	
Cog. Eng. D. R. Bratzel DRB	9/25/95	PE	
Cog. Mgr. T. J. Kelley	9/25/95	QA	
QA		Safety	
Safety		Design	
Environ.		Environ.	
Other		Other	
Proj.			
Proj.			
Proj.		DEPARTMENT OF ENERGY	
Proj.		Signature or a Control Number that tracks the Approval Signature	
		ADDITIONAL	

RELEASE AUTHORIZATION

Document Number:	WHC-SD-WM-ER-428, REV 2
Document Title:	Tank 241-BY-103 Headspace Gas and Vapor Characterization Results for Samples Collected in May 1994 and November 1994
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

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SUPPORTING DOCUMENT

1. Total Pages 42

2. Title	3. Number	4. Rev No.
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7. Abstract

Significant changes have been made to all of the original vapor characterization reports. This report documents specific headspace gas and vapor characterization results for all vapor sampling events to date. In addition, changes have been made to the original vapor reports to qualify the data based on quality assurance issues associated with the performing laboratories.

8. RELEASE STAMP

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RECORD OF REVISION	(1) Document Number WHC-SD-WM-ER-428	Page 1

(2) Title

TANK 241-BY-103 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN MAY 1994 AND NOVEMBER 1994

CHANGE CONTROL RECORD

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Revision 2
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Tank 241-BY-103 Headspace Gas and Vapor Characterization Results for Samples Collected in May 1994 and November 1994

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Contents

Acronyms and Abbreviations

CES	consensus exposure standard
EPA	Environmental Protection Agency
GC	gas chromatograph
GC/MS	gas chromatograph/mass spectrometer
ISS	*in situ* sampling
LFL	lower flammability limit
MS	mass spectrometer
NFPA	National Fire Protection Association
NPH	normal paraffinic hydrocarbon
OGIST	Oregon Graduate Institute of Science and Technology
ORNL	Oak Ridge National Laboratory
PNL	Pacific Northwest Laboratory
ppmv	parts per million by volume, 1 ppmv = 10^{-4} vol%
TNMOC	total nonmethane organic carbon
TO-14	task order 14
TST	triple sorbent trap
vol%	percent by volume, 1 vol% = 10,000 ppmv
VSS	vapor sampling system
WHC	Westinghouse Hanford Company

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Tank 241-BY-103 Headspace Gas and Vapor Characterization Results

for Samples Collected in May 1994 and November 1994

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank BY-103 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). This report primarily discusses results from the November 1994 sampling event, but also includes selected results of the May 1994 sampling event. The tank BY-103 headspace was sampled in May 1994 in accordance with *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991), and in November 1994 in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

1.2 Characterization Data Criteria

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

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). Current governing operating specifications for Watchlist tanks, such as tank BY-103, 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 BY-103 was vapor sampled in May 1994 using the *in situ* sampling (ISS) method, and again in November 1994 using the more robust vapor sampling system (VSS) method. Because the ISS sample volume flow measurement used during the May 1994 event was inherently less accurate than that of the VSS, the sorbent trap samples from the ISS event are not considered to be equivalent to those from the VSS sampling event (Huckaby et al. 1995). Furthermore, there are other discrepancies between results from the ISS and VSS methods that are not understood (Huckaby 1994a), and until the ISS method has been validated and the discrepancies resolved, results from early ISS events should be considered suspect.

Nevertheless, a brief description of the ISS event and hydrogen cyanide sampling results from the May 1994 ISS event are presented below, because this analyte was not sampled for during the VSS event. Huckaby et al. (1995) describe the bases for using the ISS method for hydrogen cyanide, and why it was not sampled for during the VSS event. Also, samples from the May 1994 ISS event were analyzed for total nonmethane organic carbon (TNMOC) by Oregon Graduate Institute of Science and Technology (OGIST), and these results are presented below because this analysis was not performed on samples from the November 1994 VSS sampling event. All other results presented here are from the November 1994 VSS 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 BY-103 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 BY-103 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

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

The cascade of tanks BY-101, BY-102, and BY-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 1994b). Changes in the concentrations of tank headspace constituents due to barometric pressure changes are consequently very slow.

2.0 SAMPLING EVENT

2.1 May 1994 *In Situ* Sampling Event

Tank BY-103 was sampled using ISS methods on May 5, 1994 by WHC Sampling and Mobile Laboratories. This sampling was conducted to satisfy requirements of *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991). Samples for hydrogen cyanide were collected from a point approximately 7.9 m below the top of the flange on riser 10B, between 2:00 p.m. and 3:00 p.m.

Huckaby et al. (1995) give a general description of the ISS method and equipment. Pingel (1994) provides field sampling information for the tank BY-103 May 1994 ISS event, and Mahon (1995) provides revised sample volume measurements. In addition to the hydrogen cyanide results presented below, Ligotke et al. (1995) and Rasmussen (1994) provide sample analysis results.

2.2 November 1994 Vapor Sampling System Sampling Event

Headspace gas and vapor samples were collected from tank BY-103 using the VSS on November 1, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-BY-103 Tank Characterization Plan* (Carpenter 1994). The tank headspace temperature was determined to be 25.5 °C. Air from the tank BY-103 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 10B, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), and Pacific Northwest Laboratories (PNL). The 32 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 11 trip blanks and 1 field blank that accompanied the samples.

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. McVeety et al. (1995) describe sample preparation and analyses.

Analyses of the VSS event inorganic vapor sorbent traps were performed within 16 days of sample collection, analyses of VSS event SUMMA™ canisters for inorganic compounds were performed 99 days after sample collection, and analyses of the ISS event hydrogen cyanide sorbent traps were performed within 57 days after sample collection (Ligotke 1995). Thus the administratively chosen 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994) was satisfied for analyses of ISS and VSS sorbent traps, but not satisfied for analyses of inorganic compounds in SUMMA™ canisters. It should be noted that these inorganic compounds (i.e., the permanent gases) would be expected to be very stable in the SUMMA™ canisters, and the results may not have been affected even though the 60-day holding time requirement had been exceeded. PNL results were produced at PNL quality assurance impact level 2, except for the hydrogen cyanide results, which were produced at PNL quality assurance impact level 3.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration in the headspace of tank BY-103 was 26 ppmv, The measured 26 ppmv of ammonia in tank BY-103 is low compared to other tanks sampled to date. Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 26 ppmv corresponds to less than 0.02 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

Hydrogen was not detected in the tank BY-103 samples, being determined to be below the limit of detection of the analytical method, 99 ppmv. In general, hydrogen is of concern as a fuel. Given the LFL of hydrogen in air to be about 4 vol%, the measured hydrogen concentration of < 99 ppmv corresponds to < 0.24 % of its LFL. At this level, hydrogen does not present a flammability concern in tank BY-103.

Nitrous oxide was measured to be an average of 16.5 ppmv in 3 SUMMA™ canister samples. Tank BY-103 has a lower nitrous oxide concentration than most of the other passively ventilated tanks that have been sampled. Under proper conditions, nitrous oxide can serve as an oxidizer to support combustion. However, Cashdollar et al. (1992) found that nitrous oxide had no significant effect on the flammability of hydrogen and air mixtures for hydrogen concentrations less than 20 vol%, and that "small amounts of nitrous oxide (relative to air) do not appear to have much effect on the flammability". Their results suggest the measured nitrous oxide concentration is much too low to have a significant effect on the flammability of the tank BY-103 headspace.

3.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 126 ppmv, is about one-third of the normal ambient air concentration, which ranges from about 350 to 400 ppmv. Lower-than-ambient carbon

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

dioxide concentrations are expected in the waste tank headspaces. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids in the waste tanks, and converted to carbonate in solution. It is reasonable to expect the level of carbon dioxide in a tank headspace will therefore depend on the tank's breathing rate, and the pH and surface area of aqueous waste (i.e., supernate, interstitial liquid, and condensate) in the tank. The 126 ppmv carbon dioxide concentration measured in tank BY-103 is typical of other tanks sampled to date.

Carbon monoxide in the tank BY-103 headspace was measured to be < 12 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. Elevated waste tank headspace carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank BY-103 headspace were determined to be $\leq$ 0.09 ppmv and $\leq$ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH waste in tank BY-103. Nitric oxide is commonly found at trace concentrations, presumably 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 BY-103 headspace. The water vapor concentration of tank BY-103 was determined to be about 11.6 mg/L, at the tank headspace temperature of 25.5 °C and pressure of 981 mbar (735.7 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 15.9 mbar (11.9 torr), to a dew point of 14.0 °C, and to a relative humidity of 49 %. The relative standard deviation of the water vapor measurements is higher than typical for this measurement.

Tritium was tested for using silica gel sorbent traps. It is assumed that tritium ions produced by the waste combine 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. Analysis of the silica gel indicated the total activity of the sample to be below the method detection limit of 50 pCi/L (WHC 1995b).

3.4 Hydrogen Cyanide

Analysis of the hydrogen cyanide specific sorbent traps indicated the concentration of this analyte to below 0.005 ppmv in all 3 samples (Ligotke et al. 1995). The absence of hydrogen cyanide at measurable concentrations is consistent with the expectation that an acid gas, such as hydrogen cyanide, would not exist at significant concentrations above the caustic waste in tank BY-103. No hydrogen cyanide has been detected in any of the 10 waste tank headspaces sampled for this analyte

3.5 Discussion of Inorganic Analytes

Aside from water and carbon dioxide, the most abundant waste constituents in the tank BY-106 headspace are ammonia and nitrous oxide. These have been detected in most tank headspaces sampled

to date, and with hydrogen, are usually the dominate waste species. The concentrations of each of these are below average for the passively ventilated tanks that have been sampled.

The relative standard deviations of the results, given in the last column in Table 3-1, are reasonable for the analytical methods used. Relative standard deviations range from 4 % for carbon dioxide and nitrous oxide, to 16 % for water vapor results. 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.), and the relative standard deviations suggest there were no significant problems in the field or in the laboratories.

4.0 ORGANIC VAPORS

Organic vapors in the tank BY-106 headspace were sampled using SUMMA™ canisters, which were analyzed at PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. None of the positively or tentatively identified organic analytes were at or above levels of concern. Both laboratories used a gas chromatograph (GC) equipped with a mass spectrometer (MS) detector to separate, identify, and quantitate the analytes. A quantitative measurement of the TNMOC concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method was also performed by OGIST on SUMMA™ canister samples from the May 1994 ISS event. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a), McVeety et al. (1995), and Rasmussen (1994).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank BY-103. These results were produced at PNL quality assurance impact level 2. All PNL analyses were not completed until 106 days after sample collection, however, and did not satisfy the administratively chosen 60-day holding time (Keller 1994). No holding time study has been performed to determine the stability of organic analytes in SUMMA™ canisters in the chemical matrix of the tank samples.

ORNL analyses of TST samples from this and other waste tanks generally agree with, support, and augment the SUMMA™ sample results. However, because certain WHC quality assurance requirements were not satisfied by ORNL, the quality assurance assessment of ORNL by Hendrickson (1995) should be reviewed before results unique to the TST samples are used for decision making.

All TSTs prepared by ORNL had 3 surrogate compounds added to evaluate sample matrix effects, potential handling, storage, and shipment problems, and analytical instrumentation performance (Jenkins et al. 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 Analytes

Positive identification of organic analytes using the methods employed by PNL and ORNL involves matching the GC retention times and MS data from a sample with that obtained 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 40 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988), plus 14 analytes selected mainly from the toxicology panel's review of vapor data on tank C-103.

Table 4-1 lists the organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL. Averages reported are from analyses of 3 SUMMA™ canister samples. PNL performed analyses

according to the EPA task order 14 (TO-14) methodology, but expanded the number of target analytes from 40 to 54 to include waste tank analytes of particular interest (EPA 1988, McVeety et al. 1995). Of the original 40 TO-14 analytes, 39 were determined to be below the 0.002 ppmv quantitation limit of the analyses, with trichlorofluoromethane being the only TO-14 analyte above its lower quantitation limit. Of the 14 additional target analytes only 2-butanone, propanone, and tetrahydrofuran were above the 0.005 ppmv method quantitation limit.

ORNL positively identified 24 of the 25 target analytes in TST samples. One target analyte, vinylidene chloride, was below the method detection limit. Despite calibration of the instrument over about a 20-fold concentration range, 18 of the 24 positively identified compounds were outside of the calibration range in at least 1 of the TST samples. The average concentrations of the positively identified compounds are given in Tables 4-2, 4-3, and 4-4. Table 4-2 lists the positively identified, quantitated analytes, Table 4-3 lists the positively identified analytes which were not quantitated, and Table 4-3 lists the positively identified analytes which exceeded their 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 Table 4-3 should not be considered quantitative and 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, butanal and 1-butanol exceeded their practical holding times, and may have been affected by the 30-day period between sample collection and analysis (Jenkins 1995b). Jenkins et al. (1995b) describe the ORNL practical holding time study, and report the practical holding times of butanal and 1-butanol are 1 and 17 days, respectively. It should be noted that the contractual holding time for the TST samples was 60 days.

Eleven target analytes were common to both the ORNL and PNL analyses. Comparison of the results from the 2 methods, which are reproduced in Table 4-5, indicates the following:

1) Both methods agree that dichloromethane, propanenitrile, n-pentanenitrile, and certain nonpolar analytes (i.e., n-hexane, n-heptane, toluene, and n-decane) are at very low levels;

2) the methods are in fair agreement for the propanone concentration; and

3) ethanenitrile at 0.026 ppmv, and n-butanenitrile at 0.090 ppmv, were found in TSTs, while analysis of SUMMA™ samples indicate these to be below their quantitation limit of 0.005 ppmv.

Though discrepancies between the TST and SUMMA™ common target analyte results are currently not understood, the measured concentrations are below levels of concern.

1-Butanol, at 2.0 ppmv, and propanone, at 0.11 to 0.49 ppmv, were the only target analytes measured to be above 0.1 ppmv. The positively identified organic compounds are neither individually nor cumulatively a flammability concern.

4.2 Tentatively Identified Organic Analytes

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 organic compounds tentatively identified in SUMMA™ canister samples by PNL are listed, with their estimated concentrations, 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 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 is particularly long and locating any given compound may be difficult, the list has been sorted alphanumerically by compound name in Table 4-8. Table 4-9 gives the same list, sorted in order of decreasing estimated concentration. Numbers in the first columns of Tables 4-8 and 4-9 (Cmpd #) identify the location of the compound in Table 4-7.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and McVeety 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. Results in these tables are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 62, 69, 80, and 85 in Table 4-7). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

4.3 Total Nonmethane Organic Carbon

OGIST measured the TNMOC concentration in 3 SUMMA™ canister samples from the May 1994 ISS event using the EPA TO-12 method (Rasmussen 1994). The sample mean was [5.2 mg/m^3], with a standard deviation of [0.4 mg/m^3]. Because OGIST did not have a WHC-approved quality assurance project plan in place at the time of analyses, OGIST data should be considered secondary data.

4.4 Discussion of Organic Analytes

Some of the compounds listed in Tables 4-1 through 4-9 were introduced to the tank with process waste streams, and are detected in the headspace because the original inventory has not been completely

evaporated or degraded. Examples of these are the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-dodecane, n-tridecane, n-tetradecane, n-pentadecane) and methyl-substituted decahydronaphthalenes that were used as diluents for tributyl phosphate.

Most of the compounds in Tables 4-1 through 4-9, however, are believed to be chemical reaction and radiolytic reaction products of the semivolatile or nonvolatile organic waste stored in the tank. 1-Butanol, for example, is known to be formed by the hydrolysis of tributyl phosphate, and it thought that the alcohols, aldehydes, ketones, nitriles, alkenes, and short chain alkanes are all degradation products of NPHs.

Neither TST nor SUMMA™ methods detected tributyl phosphate as a headspace constituent. The relatively high concentration of 1-butanol, however, is a strong indication that tributyl phosphate does exist in tank BY-103. That tributyl phosphate was not observed in the TST samples may be due to the very low vapor pressure of tributyl phosphate, and the tendency for tributyl phosphate to adsorb on the high efficiency particulate air filters used during sampling to protect the samples from radiological particulate contamination.

The tank BY-103 TST samples contained unusually high concentrations of the low volatility organic vapors. As indicated in Table 4-9, 6 of the 10 most abundant tentatively identified compounds in the TSTs have molecular formula with 14 to 16 carbon atoms. More typical for the NPH-rich tanks that have been sampled is that the semivolatile organic vapors are dominated by the much more volatile 12 and 13 carbon compounds.

5.0 SUMMARY

The tank BY-103 headspace was sampled in May 1994 and November 1994 for gases and vapors to address flammability and industrial hygiene concerns. Results unique to the May 1994 event and essentially all results from the November 1994 event have been reported. It was determined that no headspace constituents exceeded the flammability or industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

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Table 2-1
Tank BY-103 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	1.0	Organic vapors	4 tank air samples + 1 trip blank + 1 field blank
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blanks
	Oxidation bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
Tank BY-103 Inorganic Gas and Vapor Concentrations

Compound	CAS[1] Number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
Ammonia, NH_3	7664-41-7	Sorbent Trap	6	26	2	8
Carbon Dioxide, CO_2	124-38-9	SUMMA™	3	126	5	4
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 12	--	--
Hydrogen, H_2	1333-74-0	SUMMA™	3	< 99	--	--
Hydrogen Cyanide[3], HCN	74-90-8	Sorbent Trap	3	< 0.005	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.09	--	--
Nitrogen Dioxide, NO_2	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide[4], N_2O	10024-97-2	SUMMA™	3	16.5	0.7	4
Water Vapor, H_2O	7732-18-5	Sorbent Trap	6	16,200 (11.6 mg/L)	2,550 (1.8 mg/L)	16

1 CAS = Chemical Abstracts Service.

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

3 Results for hydrogen cyanide are from the May 1994 ISS event.

4 Detected in only 2 samples.

Table 4-1
Tank BY-103 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	Trichlorofluoromethane	75-69-4	0.048	0.018	37
3	Propanone (acetone)	67-64-1	0.49	0.22	45
6	2-Butanone	78-93-3	0.068	0.003	4
11	Tetrahydrofuran[4]	109-99-9	0.067	0.0004	6

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 Detected in only 2 samples.

Table 4-2
Tank BY-103 Quantitatively Measured Organic Compounds in TST Samples -- Analyses by Oak Ridge National Laboratory[1]

Cmpd #	Compound	CAS[1] Number	Average[2] (ppmv)	Standard Deviation (ppmv)	RSD[3] (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.026	0.010	38
2	Propanone (acetone)	67-64-1	0.11	0.07	67
3	2-Pentanone	107-87-9	0.019	0.013	68
4	n-Dodecane	112-40-3	0.017	0.002	12
5	n-Tridecane	629-50-5	0.029	0.003	10

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

1 CAS = Chemical Abstract Service.

2 Average of 3, 1-L TST samples.

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

Table 4-3
Tank BY-103 Positively Identified Organic Compound in TST Samples -- Analyses by Oak Ridge National Laboratory[1]

Cmpd #	Compound	CAS[2] Number	Average[3] (ppmv)	Standard Deviation (ppmv)	RSD[4] (%)
1	Dichloromethane	75-09-2	< 0.0021	--	--
2	Propanenitrile	107-12-0	< 0.0033	--	--
3	n-Hexane	110-54-3	< 0.0026	--	--
4	Benzene	71-43-2	0.0018	0.0009	49
5	n-Butanenitrile	109-74-0	0.090	0.14	156
6	n-Heptane	142-82-5	< 0.0013	--	--
7	Toluene	108-88-3	0.0015	0.0008	53
8	n-Pentanenitrile	110-59-8	< 0.0030	--	--
9	2-Hexanone	591-78-6	0.0049	0.0045	92
10	n-Octane	111-65-9	< 0.00098	--	--
11	n-Hexanenitrile	628-73-9	< 0.0018	--	--
12	2-Heptanone	110-43-0	0.0061	0.0041	67
13	n-Nonane	111-84-2	< 0.0023	--	--
14	n-Heptanenitrile	629-08-3	< 0.0036	--	--
15	2-Octanone	111-13-7	0.0020	0.0017	85
16	n-Decane	124-18-5	< 0.0054	--	--
17	n-Undecane	1120-21-4	< 0.0048	--	--

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 BY-103 Positively Identified Organic Compound 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	0.056	0.066	118
2	1-Butanol[6]	71-36-3	2.0	0.5	23

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 BY-103 Comparison of Organic Compounds in TST and SUMMA™ Samples -- Analyses by Pacific Northwest Laboratory and Oak Ridge National Laboratory

Cmpd#	Compound	CAS[1] Number	TST Average[2] (ppmv)	SUMMA™ Average[3] (ppmv)	PRD[4] (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.026	< 0.005	> 140
2	Propanone (acetone)	67-64-1	0.11	0.49	127
3	Dichloromethane	75-09-2	< 0.0021	< 0.005	--
4	Propanenitrile	107-12-0	< 0.0033	< 0.005	--
5	n-Hexane	110-54-3	< 0.0026	< 0.005	--
6	Benzene	71-43-2	0.0018	< 0.005	--
7	n-Butanenitrile	109-74-0	0.090	< 0.005	> 179
8	n-Heptane	142-82-5	< 0.0013	< 0.005	--
9	Toluene	108-88-3	0.0015	< 0.005	--
10	n-Pentanenitrile	110-59-8	< 0.0030	< 0.005	--
11	n-Decane	124-18-5	< 0.0054	< 0.005	--

1 CAS = Chemical Abstract Service.

2 Average of 3, 1-L TST samples.

3 Average of 3 sample analyses.

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

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

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m³)	Standard[3] Deviation (mg/m³)
1	Ethanol	64-17-5	0.13	0.03
2	Isopropyl Alcohol	67-63-0	0.16	0.06
3	Butanal[4]	123-72-8	0.06	--
4	1-Butanol	71-36-3	2.48	0.49
5	2-Pentanone	107-87-9	0.06	0.01
6	n-Dodecane	112-40-3	0.21	0.05
7	2,6-Dimethylundecane	17301-23-4	0.09	0.03
8	Unknown C13 Alkene/Cycloalkane		0.06	0.01
9	Unknown C14 Alkane		0.18	0.06
10	n-Tridecane	629-50-5	0.51	0.15
11	Unknown Alkane[4]		0.06	--
12	Unknown C13 Alkene/Cycloalkane		0.07	--
13	Unknown Alkane[4]		0.07	--
14	Unknown C15 Alkane		0.31	0.18
15	n-Tetradecane	629-59-4	0.55	0.29
16	Unknown Alkane[5]		0.07	0.02
17	Unknown Alkane[4]		0.07	--
18	Unknown C16 Alkane		0.38	0.17
19	Unknown C15 Alkane[4]		0.06	--
20	n-Pentadecane	629-62-9	0.22	0.03
Sum of tentatively identified compounds:			5.8	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples; presented values are estimates.

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

4 Detected in only 1 sample.

5 Detected in only 2 samples.

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

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m³)	Standard Deviation (mg/m³)
1	methyl ether	115-10-6	0.178	0.0268
2	methane, trichlorofluoro-	75-69-4	0.260	0.1377
3	2-propanol	67-63-0	0.266	0.0767
4	1-propene, 2-fluoro- and cyclopropane		0.119	0.0311
5	2-butanone	78-93-3	0.099	0.1706
6	unknown		0.030	0.0289
7	acetic acid	64-19-7	0.038	0.0424
8	1-pentanol	71-41-0	0.027	0.0233
9	methylamine, n-(1-methylbutylidene)-	22431-09-0	0.011	0.0188
10	cyclotrisiloxane, hexamethyl-	541-05-9	0.023	0.0406
11	benzene, 1,2-dimethyl- and c3-cyclopropane		0.014	0.0137
12	cyclopropane, propyl- and c2-benzene		0.010	0.0179
13	3-heptanone	106-35-4	0.042	0.0246
14	heptanal	111-71-7	0.008	0.0138
15	3-buten-2-ol	598-32-3	0.092	0.0462
16	cyclotetrasiloxane, octamethyl-	556-67-2	0.020	0.0344
17	octanal	124-13-0	0.008	0.0134
18	1-hexanol, 2-ethyl-	104-76-7	0.008	0.0141
19	pentanal, 2-methyl-	123-15-9	0.008	0.0135
20	nonanal	124-19-6	0.012	0.0216
21	benzeneacetic acid, .alpha.,4-bis[(trimethylsilyl)oxy]-,methyl ester	55334-40-2	0.022	0.0218
22	heptane, 3-ethyl-2-methyl-	14676-29-0	0.023	0.0210
23	undecane, 2-methyl-	7045-71-8	0.020	0.0190
24	undecane, 3,7-dimethyl-	17301-29-0	0.007	0.0127

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
25	cyclododecane	294-62-2	0.003	0.0057
26	cyclopentane, 1-hexyl-3-methyl-	61142-68-5	0.004	0.0061
27	decanal	112-31-2	0.010	0.0013
28	undecane, 2,6-dimethyl-	17301-23-4	0.072	0.0104
29	alkane and acetophenone, 2'-hydroxy-5'-methoxy-		0.002	0.0043
30	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.023	0.0022
31	dimethyl-decahydronaphthalene		0.005	0.0047
32	cyclohexane, hexyl-	4292-75-5	0.025	0.0046
33	dodecane, 6-methyl-	6044-71-9	0.007	0.0060
34	undecane, 2,4-dimethyl-	17312-80-0	0.008	0.0093
35	dodecane, 4-methyl-	6117-97-1	0.011	0.0100
36	dodecane, 2-methyl-	1560-97-0	0.036	0.0061
37	decane, 2,6,7-trimethyl-	62108-25-2	0.154	0.0193
38	c7-cyclohexane		0.005	0.0045
39	trimethyl-decahydronaphthalene		0.006	0.0049
40	1-tridecene	2437-56-1	0.015	0.0022
41	6-tridecene, 7-methyl-	24949-42-6	0.018	0.0056
42	1-tetradecene	1120-36-1	0.008	0.0016
43	c14-alkene		0.011	0.0018
44	decane, 2,6,7-trimethyl-	62108-25-2	0.009	0.0077
45	c13-alkene		0.006	0.0052
46	dodecane, 2,5-dimethyl-	56292-65-0	0.023	0.0202
47	c7-cyclohexane		0.003	0.0044
48	c14-alkene		0.003	0.0047
49	tridecane, 6-methyl-	13287-21-3	0.012	0.0216
50	tridecane, 6-methyl-	13287-21-3	0.016	0.0014
51	c8-cyclohexane		0.042	0.0047
52	tridecane, 4-methyl-	26717	0.028	0.0029

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
53	tridecane, 2-methyl-	1560-96-9	0.044	0.0042
54	alkyl-cyclohexane and others		0.009	0.0007
55	dodecane, 3-methyl-	17312-57-1	0.026	0.0025
56	dodecane, 2,6,10-trimethyl-	3891-98-3	0.209	0.0206
57	4-nonene, 2,3,3-trimethyl-, (Z)-	63830-68-2	0.031	0.0064
58	tetradecane	629-59-4	0.370	0.0342
59	c14-alkane		0.062	0.0056
60	tetradecane	629-59-4	0.016	0.0031
61	c14-alkane and others		0.011	0.0098
62	pentadecane	629-62-9	0.005	0.0087
63	alkane		0.003	0.0047
64	3-decanol	1565-81-7	0.018	0.0088
65	alkanol		0.038	0.0254
66	pentadecane	629-62-9	0.004	0.0066
67	alkane		0.004	0.0068
68	1-octanol, 2-butyl-	3913-02-8	0.009	0.0079
69	pentadecane	629-62-9	0.032	0.0288
70	c15-alkane		0.004	0.0073
71	c15-alkane		0.015	0.0268
72	hexadecane	544-76-3	0.136	0.1215
73	dodecane, 2-methyl-8-propyl-	55045-07-3	0.072	0.1249
74	tetradecane, 3-methyl-	18435-22-8	0.015	0.0135
75	pentadecane, 2-methyl-	1560-93-6	0.008	0.0141
76	alkane		0.006	0.0057
77	hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.009	0.0079
78	c15-alkane		0.005	0.0090
79	1-dodecyn-4-ol	74646-36-9	0.042	0.0286
80	pentadecane	629-62-9	0.259	0.0402

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
81	alkanol		0.005	0.0086
82	alkane		0.002	0.0032
83	tetradecane, 2,5-dimethyl-	56292-69-4	0.007	0.0057
84	2,3-butanediol, 2,3-dimethyl-	76-09-5	0.003	0.0052
85	pentadecane	629-62-9	0.003	0.0054
86	alkanoic acid		0.005	0.0093
87	tetradecane, 2,6,10-trimethyl-	14905-56-7	0.017	0.0151
88	pentadecane, 2,6,10-trimethyl-(nor-pristan)	3892-00-0	0.013	0.0223
89	tetradecane, 4,11-dimethyl-	55045-12-0	0.008	0.0010
90	pentadecane, 2-methyl-	1560-93-6	0.026	0.0229
91	dodecane, 2-methyl-8-propyl-	55045-07-3	0.013	0.0230
92	hexadecane	544-76-3	0.017	0.0020
93	alkane		0.007	0.0060
94	c16-alkane		0.004	0.0062
95	5-undecanone, 2-methyl-	50639-02-6	0.019	0.0017
96	alkanone		0.005	0.0090
97	tridecane, 2,5-dimethyl-	56292-66-1	0.006	0.0050
98	dodecane, 4,9-dipropyl-	3054-63-5	0.003	0.0052
99	alkanal		0.003	0.0044
100	hexadecane	544-76-3	0.113	0.0040
101	1,1'-biphenyl, 2-chloro-	2051-60-7	0.006	0.0052
102	cyclohexadecane	295-65-8	0.003	0.0050
103	phthalate		0.020	0.0026
104	dodecane, 2,6,10-trimethyl-	3891-98-3	0.010	0.0174
105	pentadecane, 2,6,10-trimethyl-(non-pristan)	3892-00-0	0.009	0.0149
106	dodecane, 4,9-dipropyl-	3054-63-5	0.013	0.0230
107	benzenamine, n-phenyl-	122-39-4	0.005	0.0045

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
108	5-tridecanone	30692-16-1	0.005	0.0085
109	heptadecane	629-78-7	0.018	0.0065
110	pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.018	0.0078
111	alkene		0.005	0.0089
112	alkane		0.003	0.0058
113	tetradecanoic acid	544-63-8	0.058	0.0210
114	eicosane	112-95-8	0.013	0.0219
115	benzenesulfonamide, n-butyl-	3622-84-2	0.055	0.0197
116	tetradecanoic acid	544-63-8	0.002	0.0033
117	pentadecanoic acid	1002-84-2	0.027	0.0123
118	1-hexadecanol	36653-82-4	0.006	0.0050
119	2-octadecenal	56554-96-2	0.008	0.0140
120	9-hexadecenoic acid	2091-29-4	0.050	0.0436
121	hexadecanoic acid	57-10-3	0.113	0.0893
122	eicosane	112-95-8	0.016	0.0283
123	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.017	0.0180
124	hexadecanoic acid	57-10-3	0.003	0.0057
125	1-hexadecene	629-73-2	0.016	0.0141
126	1-hexadecanol	36653-82-4	0.004	0.0073
127	eicosane	112-95-8	0.003	0.0052
Sum of tentatively identified compounds:			4.15	

1 CAS = Chemical Abstract Service.

2 Average of 3, 1-L TST samples; average includes samples where concentration was zero, presented values are estimates.

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

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
79	1-dodecyn-4-ol	74646-36-9	0.042	0.0286
118	1-hexadecanol	36653-82-4	0.006	0.0050
68	1-octanol, 2-butyl-	3913-02-8	0.009	0.0079
4	1-propene, 2-fluoro- and cyclopropane		0.119	0.0311
125	1-hexadecene	629-73-2	0.016	0.0141
40	1-tridecene	2437-56-1	0.015	0.0022
42	1-tetradecene	1120-36-1	0.008	0.0016
8	1-pentanol	71-41-0	0.027	0.0233
126	1-hexadecanol	36653-82-4	0.004	0.0073
18	1-hexanol, 2-ethyl-	104-76-7	0.008	0.0141
101	1,1'-biphenyl, 2-chloro-	2051-60-7	0.006	0.0052
5	2-butanone	78-93-3	0.099	0.1706
3	2-propanol	67-63-0	0.266	0.0767
119	2-octadecenal	56554-96-2	0.008	0.0140
84	2,3-butanediol, 2,3-dimethyl-	76-09-5	0.003	0.0052
13	3-heptanone	106-35-4	0.042	0.0246
15	3-buten-2-ol	598-32-3	0.092	0.0462
64	3-decanol	1565-81-7	0.018	0.0088
57	4-nonene, 2,3,3-trimethyl-, (Z)-	63830-68-2	0.031	0.0064
95	5-undecanone, 2-methyl-	50639-02-6	0.019	0.0017
108	5-tridecanone	30692-16-1	0.005	0.0085
41	6-tridecene, 7-methyl-	24949-42-6	0.018	0.0056
120	9-hexadecenoic acid	2091-29-4	0.050	0.0436
7	acetic acid	64-19-7	0.038	0.0424
99	alkanal		0.003	0.0044

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
29	alkane and acetophenone, 2'-hydroxy-5'-methoxy-		0.002	0.0043
63	alkane		0.003	0.0047
67	alkane		0.004	0.0068
76	alkane		0.006	0.0057
82	alkane		0.002	0.0032
93	alkane		0.007	0.0060
112	alkane		0.003	0.0058
86	alkanoic acid		0.005	0.0093
65	alkanol		0.038	0.0254
81	alkanol		0.005	0.0086
96	alkanone		0.005	0.0090
111	alkene		0.005	0.0089
54	alkyl-cyclohexane and others		0.009	0.0007
107	benzenamine, n-phenyl-	122-39-4	0.005	0.0045
11	benzene, 1,2-dimethyl- and c3-cyclopropane		0.014	0.0137
21	benzeneacetic acid, .alpha.,4-bis[(trimethylsilyl)oxy]-,methyl ester	55334-40-2	0.022	0.0218
115	benzenesulfonamide, n-butyl-	3622-84-2	0.055	0.0197
45	c13-alkene		0.006	0.0052
43	c14-alkene		0.011	0.0018
48	c14-alkene		0.003	0.0047
59	c14-alkane		0.062	0.0056
61	c14-alkane and others		0.011	0.0098
78	c15-alkane		0.005	0.0090
71	c15-alkane		0.015	0.0268
70	c15-alkane		0.004	0.0073
94	c16-alkane		0.004	0.0062
38	c7-cyclohexane		0.005	0.0045

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
47	c7-cyclohexane		0.003	0.0044
51	c8-cyclohexane		0.042	0.0047
25	cyclododecane	294-62-2	0.003	0.0057
102	cyclohexadecane	295-65-8	0.003	0.0050
30	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.023	0.0022
32	cyclohexane, hexyl-	4292-75-5	0.025	0.0046
26	cyclopentane, 1-hexyl-3-methyl-	61142-68-5	0.004	0.0061
12	cyclopropane, propyl- and c2-benzene		0.010	0.0179
16	cyclotetrasiloxane, octamethyl-	556-67-2	0.020	0.0344
10	cyclotrisiloxane, hexamethyl-	541-05-9	0.023	0.0406
27	decanal	112-31-2	0.010	0.0013
37	decane, 2,6,7-trimethyl-	62108-25-2	0.154	0.0193
44	decane, 2,6,7-trimethyl-	62108-25-2	0.009	0.0077
31	dimethyl-decahydronaphthalene		0.005	0.0047
33	dodecane, 6-methyl-	6044-71-9	0.007	0.0060
35	dodecane, 4-methyl-	6117-97-1	0.011	0.0100
36	dodecane, 2-methyl-	1560-97-0	0.036	0.0061
46	dodecane, 2,5-dimethyl-	56292-65-0	0.023	0.0202
55	dodecane, 3-methyl-	17312-57-1	0.026	0.0025
56	dodecane, 2,6,10-trimethyl-	3891-98-3	0.209	0.0206
73	dodecane, 2-methyl-8-propyl-	55045-07-3	0.072	0.1249
91	dodecane, 2-methyl-8-propyl-	55045-07-3	0.013	0.0230
98	dodecane, 4,9-dipropyl-	3054-63-5	0.003	0.0052
104	dodecane, 2,6,10-trimethyl-	3891-98-3	0.010	0.0174
106	dodecane, 4,9-dipropyl-	3054-63-5	0.013	0.0230
114	eicosane	112-95-8	0.013	0.0219
122	eicosane	112-95-8	0.016	0.0283
127	eicosane	112-95-8	0.003	0.0052

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
109	heptadecane	629-78-7	0.018	0.0065
14	heptanal	111-71-7	0.008	0.0138
22	heptane, 3-ethyl-2-methyl-	14676-29-0	0.023	0.0210
72	hexadecane	544-76-3	0.136	0.1215
77	hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.009	0.0079
92	hexadecane	544-76-3	0.017	0.0020
100	hexadecane	544-76-3	0.113	0.0040
121	hexadecanoic acid	57-10-3	0.113	0.0893
123	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.017	0.0180
124	hexadecanoic acid	57-10-3	0.003	0.0057
2	methane, trichlorofluoro-	75-69-4	0.260	0.1377
1	methyl ether	115-10-6	0.178	0.0268
9	methylamine, n-(1-methylbutylidene)-	22431-09-0	0.011	0.0188
20	nonanal	124-19-6	0.012	0.0216
17	octanal	124-13-0	0.008	0.0134
62	pentadecane	629-62-9	0.005	0.0087
66	pentadecane	629-62-9	0.004	0.0066
69	pentadecane	629-62-9	0.032	0.0288
75	pentadecane, 2-methyl-	1560-93-6	0.008	0.0141
80	pentadecane	629-62-9	0.259	0.0402
85	pentadecane	629-62-9	0.003	0.0054
88	pentadecane, 2,6,10-trimethyl- (nor-pristan)	3892-00-0	0.013	0.0223
90	pentadecane, 2-methyl-	1560-93-6	0.026	0.0229
105	pentadecane, 2,6,10-trimethyl- (non-pristan)	3892-00-0	0.009	0.0149
110	pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.018	0.0078
117	pentadecanoic acid	1002-84-2	0.027	0.0123
19	pentanal, 2-methyl-	123-15-9	0.008	0.0135
103	phthalate		0.020	0.0026

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
58	tetradecane	629-59-4	0.370	0.0342
60	tetradecane	629-59-4	0.016	0.0031
74	tetradecane, 3-methyl-	18435-22-8	0.015	0.0135
83	tetradecane, 2,5-dimethyl-	56292-69-4	0.007	0.0057
87	tetradecane, 2,6,10-trimethyl-	14905-56-7	0.017	0.0151
89	tetradecane, 4,11-dimethyl-	55045-12-0	0.008	0.0010
113	tetradecanoic acid	544-63-8	0.058	0.0210
116	tetradecanoic acid	544-63-8	0.002	0.0033
49	tridecane, 6-methyl-	13287-21-3	0.012	0.0216
50	tridecane, 6-methyl-	13287-21-3	0.016	0.0014
52	tridecane, 4-methyl-	26717	0.028	0.0029
53	tridecane, 2-methyl-	1560-96-9	0.044	0.0042
97	tridecane, 2,5-dimethyl-	56292-66-1	0.006	0.0050
39	trimethyl-decahydronaphthalene		0.006	0.0049
23	undecane, 2-methyl-	7045-71-8	0.020	0.0190
24	undecane, 3,7-dimethyl-	17301-29-0	0.007	0.0127
28	undecane, 2,6-dimethyl-	17301-23-4	0.072	0.0104
34	undecane, 2,4-dimethyl-	17312-80-0	0.008	0.0093
6	unknown		0.030	0.0289
Sum of tentatively identified compounds:			4.15	

1 CAS = Chemical Abstract Service.

2 Average of 3, 1-L TST samples; average includes samples where concentration was zero; presented values are estimates.

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

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
58	tetradecane	629-59-4	0.370	0.0342
3	2-propanol	67-63-0	0.266	0.0767
2	methane, trichlorofluoro-	75-69-4	0.260	0.1377
80	pentadecane	629-62-9	0.259	0.0402
56	dodecane, 2,6,10-trimethyl-	3891-98-3	0.209	0.0206
1	methyl ether	115-10-6	0.178	0.0268
37	decane, 2,6,7-trimethyl-	62108-25-2	0.154	0.0193
72	hexadecane	544-76-3	0.136	0.1215
121	hexadecanoic acid	57-10-3	0.113	0.0893
100	hexadecane	544-76-3	0.113	0.0040
5	2-butanone	78-93-3	0.099	0.1706
15	3-buten-2-ol	598-32-3	0.092	0.0462
28	undecane, 2,6-dimethyl-	17301-23-4	0.072	0.0104
73	dodecane, 2-methyl-8-propyl-	55045-07-3	0.072	0.1249
59	c14-alkane		0.062	0.0056
113	tetradecanoic acid	544-63-8	0.058	0.0210
115	benzenesulfonamide, n-butyl-	3622-84-2	0.055	0.0197
120	9-hexadecenoic acid	2091-29-4	0.050	0.0436
53	tridecane, 2-methyl-	1560-96-9	0.044	0.0042
13	3-heptanone	106-35-4	0.042	0.0246
51	c8-cyclohexane		0.042	0.0047
79	1-dodecyn-4-ol	74646-36-9	0.042	0.0286
7	acetic acid	64-19-7	0.038	0.0424
65	alkanol		0.038	0.0254
36	dodecane, 2-methyl-	1560-97-0	0.036	0.0061
69	pentadecane	629-62-9	0.032	0.0288

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
4	1-propene, 2-fluoro- and cyclopropane		0.119	0.0311
57	4-nonene, 2,3,3-trimethyl-, (Z)-	63830-68-2	0.031	0.0064
6	unknown		0.030	0.0289
52	tridecane, 4-methyl-	26717	0.028	0.0029
8	1-pentanol	71-41-0	0.027	0.0233
117	pentadecanoic acid	1002-84-2	0.027	0.0123
90	pentadecane, 2-methyl-	1560-93-6	0.026	0.0229
55	dodecane, 3-methyl-	17312-57-1	0.026	0.0025
32	cyclohexane, hexyl-	4292-75-5	0.025	0.0046
46	dodecane, 2,5-dimethyl-	56292-65-0	0.023	0.0202
22	heptane, 3-ethyl-2-methyl-	14676-29-0	0.023	0.0210
30	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.023	0.0022
10	cyclotrisiloxane, hexamethyl-	541-05-9	0.023	0.0406
21	benzeneacetic acid, .alpha.,4-bis[(trimethylsilyl)oxy]-,methyl ester	55334-40-2	0.022	0.0218
16	cyclotetrasiloxane, octamethyl-	556-67-2	0.020	0.0344
23	undecane, 2-methyl-	7045-71-8	0.020	0.0190
103	phthalate		0.020	0.0026
95	5-undecanone, 2-methyl-	50639-02-6	0.019	0.0017
41	6-tridecene, 7-methyl-	24949-42-6	0.018	0.0056
110	pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.018	0.0078
109	heptadecane	629-78-7	0.018	0.0065
64	3-decanol	1565-81-7	0.018	0.0088
12	cyclopropane, propyl- and c2-benzene		0.010	0.0179
92	hexadecane	544-76-3	0.017	0.0020
87	tetradecane, 2,6,10-trimethyl-	14905-56-7	0.017	0.0151
123	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.017	0.0180
50	tridecane, 6-methyl-	13287-21-3	0.016	0.0014
125	1-hexadecene	629-73-2	0.016	0.0141

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
60	tetradecane	629-59-4	0.016	0.0031
122	eicosane	112-95-8	0.016	0.0283
71	c15-alkane		0.015	0.0268
40	1-tridecene	2437-56-1	0.015	0.0022
74	tetradecane, 3-methyl-	18435-22-8	0.015	0.0135
11	benzene, 1,2-dimethyl- and c3-cyclopropane		0.014	0.0137
114	eicosane	112-95-8	0.013	0.0219
88	pentadecane, 2,6,10-trimethyl-(nor-pristan)	3892-00-0	0.013	0.0223
91	dodecane, 2-methyl-8-propyl-	55045-07-3	0.013	0.0230
106	dodecane, 4,9-dipropyl-	3054-63-5	0.013	0.0230
49	tridecane, 6-methyl-	13287-21-3	0.012	0.0216
20	nonanal	124-19-6	0.012	0.0216
61	c14-alkane and others		0.011	0.0098
9	methylamine, n-(1-methylbutylidene)-	22431-09-0	0.011	0.0188
35	dodecane, 4-methyl-	6117-97-1	0.011	0.0100
43	c14-alkene		0.011	0.0018
104	dodecane, 2,6,10-trimethyl-	3891-98-3	0.010	0.0174
27	decanal	112-31-2	0.010	0.0013
105	pentadecane, 2,6,10-trimethyl-(non-pristan)	3892-00-0	0.009	0.0149
54	alkyl-cyclohexane and others		0.009	0.0007
68	1-octanol, 2-butyl-	3913-02-8	0.009	0.0079
44	decane, 2,6,7-trimethyl-	62108-25-2	0.009	0.0077
77	hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.009	0.0079
75	pentadecane, 2-methyl-	1560-93-6	0.008	0.0141
14	heptanal	111-71-7	0.008	0.0138
18	1-hexanol, 2-ethyl-	104-76-7	0.008	0.0141
42	1-tetradecene	1120-36-1	0.008	0.0016
119	2-octadecenal	56554-96-2	0.008	0.0140

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
17	octanal	124-13-0	0.008	0.0134
19	pentanal, 2-methyl-	123-15-9	0.008	0.0135
34	undecane, 2,4-dimethyl-	17312-80-0	0.008	0.0093
89	tetradecane, 4,11-dimethyl-	55045-12-0	0.008	0.0010
83	tetradecane, 2,5-dimethyl-	56292-69-4	0.007	0.0057
33	dodecane, 6-methyl-	6044-71-9	0.007	0.0060
24	undecane, 3,7-dimethyl-	17301-29-0	0.007	0.0127
93	alkane		0.007	0.0060
39	trimethyl-decahydronaphthalene		0.006	0.0049
118	1-hexadecanol	36653-82-4	0.006	0.0050
101	1,1'-biphenyl, 2-chloro-	2051-60-7	0.006	0.0052
45	c13-alkene		0.006	0.0052
76	alkane		0.006	0.0057
97	tridecane, 2,5-dimethyl-	56292-66-1	0.006	0.0050
96	alkanone		0.005	0.0090
86	alkanoic acid		0.005	0.0093
107	benzenamine, n-phenyl-	122-39-4	0.005	0.0045
81	alkanol		0.005	0.0086
31	dimethyl-decahydronaphthalene		0.005	0.0047
38	c7-cyclohexane		0.005	0.0045
78	c15-alkane		0.005	0.0090
62	pentadecane	629-62-9	0.005	0.0087
111	alkene		0.005	0.0089
108	5-tridecanone	30692-16-1	0.005	0.0085
29	alkane and acetophenone, 2'-hydroxy-5'-methoxy-		0.002	0.0043
67	alkane		0.004	0.0068
66	pentadecane	629-62-9	0.004	0.0066
94	c16-alkane		0.004	0.0062

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
70	c15-alkane		0.004	0.0073
26	cyclopentane, 1-hexyl-3-methyl-	61142-68-5	0.004	0.0061
126	1-hexadecanol	36653-82-4	0.004	0.0073
48	c14-alkene		0.003	0.0047
47	c7-cyclohexane		0.003	0.0044
112	alkane		0.003	0.0058
63	alkane		0.003	0.0047
84	2,3-butanediol, 2,3-dimethyl-	76-09-5	0.003	0.0052
85	pentadecane	629-62-9	0.003	0.0054
102	cyclohexadecane	295-65-8	0.003	0.0050
98	dodecane, 4,9-dipropyl-	3054-63-5	0.003	0.0052
99	alkanal		0.003	0.0044
127	eicosane	112-95-8	0.003	0.0052
124	hexadecanoic acid	57-10-3	0.003	0.0057
25	cyclododecane	294-62-2	0.003	0.0057
82	alkane		0.002	0.0032
116	tetradecanoic acid	544-63-8	0.002	0.0033
Sum of tentatively identified compounds:			4.15	

1 CAS = Chemical Abstract Service.

2 Average of 3, 1-L TST samples; average includes samples where concentration was zero; presented values are estimates.

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