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Title/Desc:

TANK 241BY110 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
11/1994

COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 21. ECN **№ 625443**Proj.
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Page 2 of 2

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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.

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Document Number Revision

20. Approvals

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Cog. Eng. D. R. Bratzel <i>DR Bratzel</i>	9/25/95	PE	_____
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Other	_____	Other	_____
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	_____	Signature or a Control Number that tracks the Approval Signature	

	_____	<u>ADDITIONAL</u>	

RELEASE AUTHORIZATION

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Characterization Results for Samples Collected in
November 1994

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

APPROVED FOR PUBLIC RELEASE

WHC Information Release Administration Specialist:

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9/26/95

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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.		
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Tank 241-BY-110 Headspace Gas and Vapor Characterization Results for Samples Collected in November 1994

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Contents

1.0 INTRODUCTION	1
1.1 Characterization Objectives	1
1.2 Characterization Data Criteria	1
1.3 Sampling Overview	2
1.4 Tank Headspace Dynamics	2
2.0 SAMPLING EVENT	3
3.0 INORGANIC GASES AND VAPORS	4
3.1 Ammonia, Hydrogen, and Nitrous Oxide	4
3.2 Carbon Dioxide and Carbon Monoxide	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 Analytes	7
4.2 Tentatively Identified Organic Analytes	8
4.4 Discussion of Organic Analytes	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

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Tank 241-BY-110 Headspace Gas and Vapor Characterization Results
for Samples Collected in November 1994

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank BY-110 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. 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 BY-110 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). Current governing operating specifications for Watchlist tanks, such as tank BY-110, 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 representative of the tank BY-110 headspace when the tank was sampled, and sample analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents (Meacham et al. 1995). No assessment has been made of how the tank BY-110 headspace composition changes with time, though studies of tank C-103 suggest that composition changes probably occur very slowly in the passively ventilated tanks (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank BY-110 is the first tank in a 3-tank cascade with tanks BY-111 and BY-112. It is connected to tank BY-111 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long cascade line. Tanks BY-111 and BY-112 are also 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-111 or BY-112 may be transferred to tank BY-110 (unless the cascade lines are obstructed).

The cascade of tanks BY-110, BY-111, and BY-112 is passively ventilated, which means that the tanks are allowed to exhale air, waste gases, and vapors as the barometric pressure falls, and inhale ambient air as the barometric pressure rises. Each of these tanks has its own filtered breather riser. Barometric pressure typically rises and falls on a diurnal cycle, producing an average daily exchange of air equal to about 0.46 % of each tank headspace (Huckaby 1994). Changes in the concentrations of tank headspace constituents due to barometric pressure changes are consequently very slow.

2.0 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank BY-110 using the vapor sampling system (VSS) on November 11, 1994 by WHC Sampling and Mobile Laboratories, (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-BY-110 Tank Characterization Plan* (Carpenter 1994). The tank headspace temperature was determined to be 27 °C. Air from the tank BY-110 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 12B, 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 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 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^{TM,1} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions as given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM canisters were prepared and analyzed by PNL at PNL quality assurance impact level 2. Clauss et al. (1995) describe sample preparation and analyses.

Analyses of the VSS event inorganic vapor sorbent traps were performed within 39 days of sample collection, analyses of VSS event SUMMATM canisters for inorganic compounds were performed 70 days after sample collection (Ligothe 1995). Thus the 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994) was satisfied for analyses of VSS sorbent traps, but not for SUMMATM sample analyses. It should be noted that these inorganic compounds (i.e., the permanent gases) would be expected to be very stable in the SUMMATM canisters, and the results may not have been affected even though the administratively chosen 60-day holding time requirements were exceeded. No holding time study has been performed to determine the stability of the inorganic analytes in SUMMATM canisters in the chemical matrix of the tank samples.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Ammonia concentration in the headspace of tank BY-110 was measured to be 401 ppmv. Ammonia is thought to be a product of chemical and radiolytic waste degradation processes. It has been observed in virtually all of the waste tanks sampled to date, at concentrations ranging from about 3 ppmv in C-108 (Lucke et al. 1995), to 1040 ppmv in tank BY-108 (McVeety et al. 1995). Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 401 ppmv corresponds to less than 0.3 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

Hydrogen was not detected in the tank BY-110 samples, being determined to be below the limit of detection of the analytical method, 160 ppmv. In general, hydrogen is of concern as a fuel. The 160 ppmv detection limit corresponds to about 0.4 % of the lower LFL for hydrogen in air.

The average nitrous oxide concentration measured in the 3 SUMMATM canister samples was 103 ppmv. Nitrous oxide is commonly found in the passively ventilated waste tanks, and the 103 ppmv concentration in tank BY-110 is about average for the 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-110 headspace.

3.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 229 ppmv, is significantly less than the normal ambient air concentration of 350 to 400 ppmv. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. It is reasonable to expect the level of carbon dioxide in a tank headspace will therefore depend on the tank's breathing rate, and the pH and surface area of aqueous

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

waste (i.e., supernate, interstitial liquid, and condensate) in the tank. The 229 ppmv carbon dioxide concentration measured in tank BY-110 is typical of other tanks that have been sampled.

Carbon monoxide in the tank BY-110 headspace, measured to be < 76 ppmv, is not well characterized. The method quantitation limit, 76 ppmv, is above the highest waste tank carbon monoxide concentration measured to date ([26.7 ppmv] in tank C-103², Huckaby and Story 1994).

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank BY-110 headspace were determined to be $\leq$ 0.09 ppmv and $\leq$ 0.05 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH waste in tank BY-110. 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-110 headspace.

The water vapor concentration was measured by gravimetric analysis of 5 sorbent trap systems by PNL (Clauss et al. 1995). The water vapor concentration of tank BY-110 was determined to be about 8.0 mg/L, at the tank headspace temperature of 27 °C and pressure of 985 mbar (739.2 torr). This corresponds to a water vapor partial pressure of 11.1 mbar (8.3 torr), to a dew point of 8.5 °C, and to a relative humidity of 31%.

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

3.4 Discussion of Inorganic Gases and Vapors

Aside from water vapor and carbon dioxide, the most abundant waste constituents in the tank BY-110 headspace are ammonia and nitrous oxide. These have been detected in most tank headspaces that have been sampled, and along with hydrogen, are usually the dominate waste species.

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 2 % for water vapor, to 23 % for carbon dioxide 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.

As discussed briefly in Section 1.4, it is possible that gases and vapors generated by the waste in tanks BY-111 and BY-112 could be transferred to tank BY-110 via the cascade lines. If significant exchange of selected inorganic gases and vapors were taking place between adjacent tanks, either their headspace compositions would be very similar, or all constituents detected in one tank would be at or equal or higher

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.

concentrations in the other tank. The data in Table 3-2 are consistent with the premise that air, gases, and vapors could be transferring from tank BY-111 to tank BY-110 (waste species are at higher concentrations in tank BY-110 than in BY-111), but do not constitute proof that this is occurring.

4.0 ORGANIC VAPORS

Organic vapors in the tank BY-110 headspace were sampled using SUMMA™ canisters, which were analyzed at PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Both laboratories used a gas chromatograph (GC) equipped with a mass spectrometer (MS) to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Clauss et al. (1995).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank BY-110. These results were produced at PNL quality assurance impact level 2: However, PNL analyses of organic vapors in SUMMA™ canisters were not completed until 76 days after sample collection (Ligothe 1995), and exceeded the administratively chosen 60-day holding time specified by the WHC quality assurance project plan (Keller 1994). No holding time study has been performed to determine the stability of the organic analytes in SUMMA™ in the chemical matrix of the tank air 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 39 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988), plus 14 analytes selected mainly from the toxicology panel's review of vapor data on tank C-103.

Given in Table 4-1 are 13 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 55 to include waste tank analytes of particular interest (EPA 1988, Clauss et al. 1995). Of the original 40 TO-14 analytes, only trichlorofluoromethane and 1,2,4-trichlorobenzene were determined to be above the 0.002 ppmv quantitation limit of the analyses (Clauss et al. 1995 provide the complete TO-

14 analyte list). Five of the 15 additional target analytes (1-propanol, acetonitrile, butanal, propanenitrile, and butanenitrile) were below the 0.005 ppmv method quantitation limit.

ORNL positively identified 23 of 27 target analytes selected by WHC. Four target analytes (vinylidene chloride, dichloromethane, tributyl phosphate and dibutyl butylphosphonate) were below detection limits. Five detected and quantitated analytes, and their average concentrations from the analysis of 3 TSTs, are given in Table 4-2. Despite calibration of the instrument over about a 20-fold concentration range, 16 of the 23 compounds were outside of the calibration range in at least 1 of the TST samples. Table 4-3 lists 13 of the positively identified analytes which were not quantitated. Table 4-4 lists the remaining positively identified analytes, 2 of which were quantitated and 3 of which were not quantitated, that exceeded the ORNL analyte-specific practical holding times. Data in Tables 4-3 and 4-4 may not be accurate to within $\pm 30\%$ as specified by Burnum (1995).

Based on a practical holding time study performed by ORNL the reported concentrations of propanone, butanal, 1-butanol, 2-pentanone, and n-pentanenitrile may have been affected by the 60-day period between sample collection and analysis (Jenkins 1995b). The concentration of these five analytes are reported in Table 4-4. The practical holding time is defined as the holding time for which there is a 15 % risk that the concentration of an analyte in the sample will be below its initial concentration. Jenkins et al (1995b) describe the ORNL practical holding time study, and report practical holding times for these compounds. It should be noted, however, that the contractual holding time for the TST samples was 60-days.

Twelve target analytes that were common to both the ORNL and PNL analyses are listed in Table 4-5. Two of these, dichloromethane and vinylidene chloride, were not detected by either laboratory. Comparison of the results for the other 10 analytes from the 2 laboratories indicates the following:

- 1) The methods agree well on the concentrations of n-heptane and n-decane;
- 2) the methods are in fair agreement on the concentration of acetone, with TST analysis indicating 3.8 ppmv, and SUMMATM analysis indicating 9.9 ppmv;
- 3) n-hexane was detected by both methods, but the agreement is poor, with TST analysis indicating 0.29 ppmv, and SUMMATM analysis indicating 0.017 ppmv; and
- 4) ethanenitrile, propanenitrile, butanal, benzene, n-butanenitrile, and toluene were reported to be below SUMMATM analysis method quantitation limits, yet each of these were measured in TST samples to be significantly above the SUMMATM method quantitation limits.

Though the discrepancies between the TST and SUMMATM sample results exceed accuracy requirements specified in *Tank 241-BY-110 Tank Characterization Plan* (Carpenter 1994), benzene is the only analyte in question that exceeds the action limit specified by *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

The most abundant analytes in Tables 4-1 through 4-4 are propanone, ethanenitrile, and 2-butanone. At the reported concentrations, these analytes do not individually or cumulatively represent a flammability hazard.

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 SUMMATM samples. Analyses of the samples are designed to recover, separate, and identify the organic vapors in the samples. TSTs are not good for collecting highly volatile compounds (*i.e.*, molecules more volatile than propane), but are quite good for most others. In contrast, the recovery of very low volatility compounds (*i.e.*, molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (*i.e.*, butanal) from SUMMATM samples has been problematic.

The PNL list of tentatively identified compounds, with estimated concentrations, is given in Table 4-6, and the ORNL list of tentatively identified compounds, and their estimated concentrations, is given in Table 4-7. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

Because the list of tentatively identified organic compounds in TST samples is especially long and locating any 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 elution order 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 Clauss et al. (1995), respectively, and should be reviewed before this data are used for decision making. Results in Tables 4-6 through 4-9 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks, or the assignment of the same identity to different peaks (*e.g.*, Cmpd # 22 and 41 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.

Concentrations given in Tables 4-6 through 4-9 should be considered rough estimates. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

4.4 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 in tank BY-110 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.

Though there is no toxicological or flammability hazard associated with the 0.34 ppmv of trichlorofluoromethane measured in SUMMATM canister samples from tank BY-110, its presence warrants an explanation. The origin of trichlorofluoromethane in the waste tanks has not been established, however, it is possible that it was introduced to the tank and the concrete pits of the tank through its use in urethane sealing foam.

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

Neither TST nor SUMMATM 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-110. That tributyl phosphate was not observed in the TST samples may be due to the facts that tributyl phosphate has a very low vapor pressure and is consequently present at a very low concentration, and it has a tendency to adsorb on to the high efficiency particulate air (HEPA) filters used during sampling to protect the samples from radiological particulate contamination.

Volatile alkanes and alkenes are more prominent in the tank BY-110 headspace than is typical of NPH-rich tanks. For example, n-butane has the highest estimated concentration of any the tentatively identified analyte in both SUMMATM samples (Table 4-6) and TST samples (Table 4-7). Also, the other tentatively identified analytes in SUMMATM samples with concentrations above 1 mg/m³ are propene, propane, n-pentane, and 2-methylpentane.

In the semivolatile region of Table 4-7, subjectively defined here as those compounds eluting after n-decane (Cmpd # 56 through 111), there are many branched alkanes. The abundance of these, as well as the methyl-substituted decahydronaphthalenes, has also been noted in other 241-BY farm tanks. ORNL estimated the total organic vapor concentration of tank BY-110, based on quantitative and estimated MS data, to be 29 mg/m³.

5.0 SUMMARY

The tank BY-110 headspace was sampled in November 1994 for gases and vapors to address flammability and industrial hygiene concerns. Collection and analysis of samples has been reported. It was determined that no headspace constituents exceeded the flammability notification limits, but ammonia, measured to be present at 401 ppmv, exceeded the industrial hygiene notification limit of 150 ppmv specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

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Table 2-1
Tank BY-110 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	0.05	Organic vapors	4 tank air samples
		0.25	Organic vapors	4 tank air samples
		0.50	Organic vapors	4 tank air samples + 2 trip blank + 2 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
	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
Tank BY-110 Inorganic Gas and Vapor Concentrations
Analyses by Pacific Northwest Laboratory

Compound	CAS ¹ number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	401	15	4
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	229	53	23
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 76	—	—
Hydrogen, H ₂	1333-74-0	SUMMA™	3	< 160	—	—
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.09	—	—
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.05	—	—
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	103	22	21
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	11,300 (8.0 mg/L)	250 (0.2 mg/L)	2

1 CAS = Chemical Abstracts Service.

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

Table 3-2
Comparison of Tank BY-110, BY-111, and BY-112 Headspace Constituents¹

Tank:	BY-110	BY-111 ²	BY-112 ³
Date sampled, (mo/day/yr)	11/11/94	5/11/94 11/16/94	11/18/94
Headspace temperature, (°C)	27	27	23.2
Ammonia, (ppmv)	401	59	63
Hydrogen, (ppmv)	< 160	< 160	< 94
Carbon dioxide, (ppmv)	229	219	121
Carbon monoxide, (ppmv)	< 76	< 76	< 12
Nitric oxide, (ppmv)	± 0.09	± 0.15	0.18
Nitrogen dioxide, (ppmv)	± 0.05	± 0.05	± 0.02
Nitrous oxide, (ppmv)	103	< 67	40
Water vapor, (mg/m ³)	8.0	6.9	11.2
Water vapor, (% relative humidity)	31	27	53
Ethanenitrile (acetonitrile), (ppmv)	0.81	0.050	0.10
Propanone (acetone), (ppmv)	(3.8)	(0.48)	(1.0)
1-Butanol, (ppmv)	0.30	< 0.0011	0.059
n-Dodecane, (ppmv)	0.079	< 0.00046	0.0097
n-Tridecane, (ppmv)	0.13	(0.0015)	0.020
Total organic compounds ⁴ , (mg/m ³)	29	2.2	5.8

1 Inorganic gas or vapor results are from PNL; organic vapor results are from ORNL, with semiquantitative values in parentheses and quantitative values not in parentheses.

2 Data are from Huckaby and Bratzel 1995a.

3 Data are from Huckaby and Bratzel 1995b.

4 Total organic compound concentration was estimated from TST sample results.

Table 4-1
 Tank BY-110 Quantitatively Measured Organic Compounds in SUMMA™ Samples --
 Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
1	Trichlorofluoromethane	75-69-4	0.34	0.06	18
2	Propanone (acetone)	67-64-1	9.9	2.5	25
3	2-Butanone	78-93-3	0.48	0.01	3
4	n-Hexane	110-54-3	0.017	0.017	96
5	4-Methyl-2-pentanone	108-10-1	0.0097	0.0006	7
6	Cyclohexane	110-82-7	0.021	0.003	13
7	n-Heptane	142-82-5	0.11	0.003	2
8	Tetrahydrofuran	109-99-9	0.15	0.002	1
9	Cyclohexanone ³	108-94-1	0.057	--	--
10	1,2,4-Trichlorobenzene	120-82-1	0.0159	0.0002	1
11	Pyridine	110-86-1	0.043	0.002	5
12	n-Decane	124-18-5	0.032	0.003	9
13	Methane	74-82-8	< 61	--	--

1 CAS = Chemical Abstract Service.

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

3 Detected in only 1 sample.

Table 4-2
 Tank BY-110 Quantitatively Measured Organic Compounds in TST Samples --
 Analyses by Oak Ridge National Laboratory¹

Cmpd#	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.81	0.04	5
2	n-Hexane	110-54-3	0.29	0.05	18
3	n-Heptane	142-82-5	0.15	0.03	20
4	n-Dodecane	112-40-3	0.079	0.012	15
5	n-Tridecane	629-50-5	0.13	0.004	3

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

2 CAS = Chemical Abstract Service.

3 Average of 4 TST samples by ORNL: 3 were 250 ml and 1 was 50 ml.

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

Table 4-3
 Tank BY-110 Positively Identified Organic Compounds in TST Samples --
 Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Propanenitrile	107-12-0	0.025	0.001	4
2	Benzene	71-43-2	0.034	0.01	7
3	n-Butanenitrile	109-74-0	0.028	0.008	28
4	Toluene	108-88-3	0.029	0.006	20
5	2-Hexanone	591-78-6	0.063	0.012	19
6	n-Octane	111-65-9	0.061	0.008	14
7	n-Hexanenitrile	628-73-9	0.0058	0.0009	16
8	2-Heptanone	110-43-0	0.056	0.008	14
9	n-Nonane	111-84-2	0.030	0.005	15
10	n-Heptanenitrile	629-08-3	0.0057	0.0013	23
11	2-Octanone	111-13-7	0.010	0.001	10
12	n-Decane	124-18-5	0.024	0.005	21
13	n-Undecane	1120-21-4	0.042	0.008	19

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

2 CAS = Chemical Abstract Service.

3 Average of 4 TST samples by ORNL; 3 were 250 ml and 1 was 50 ml.

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

Table 4-4
Tank BY-110 Positively Identified Organic Compounds in TST Samples
for which Practical Holding Times were Exceeded --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Propanone (acetone) ⁵	67-64-1	3.8	0.3	8
2	Butanal ⁵	123-72-8	0.036	0.007	19
3	1-Butanol ⁶	71-36-3	0.30	0.02	8
4	2-Pentanone ⁶	107-87-9	0.14	0.03	20
5	n-Pentanenitrile ⁵	110-59-8	0.0068	0.0011	16

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

2 CAS = Chemical Abstract Service.

3 Average of 4 TST samples by ORNL: 3 were 250 ml and 1 was 50 ml.

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

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

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

Table 4-5
 Tank BY-110 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 (%)
Ethanenitrile (acetonitrile)	75-05-8	0.81	< 0.005	> 198
Propanone (acetone)	67-64-1	3.8	9.9	89
Propanenitrile	107-12-0	0.025	< 0.005	> 133
Butanal	123-72-8	0.036	< 0.005	> 151
n-Hexane	110-54-3	0.29	0.017	178
Benzene	71-43-2	0.034	< 0.005	> 149
n-Butanenitrile	109-74-0	0.028	< 0.005	> 139
n-Heptane	142-82-5	0.15	0.11	31
Toluene	108-88-3	0.029	< 0.005	> 141
n-Decane	124-18-5	0.024	0.032	28

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples by ORNL: 3 were 250 ml and 1 was 50 ml.

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 BY-110 Tentatively Identified Organic Compounds
 Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Propene	115-07-1	1.70	0.58
2	Propane	74-98-6	1.12	0.44
3	Cyclopropane	75-19-4	0.26	0.08
4	Isobutane	75-28-5	0.54	0.17
5	1-Butene	106-98-9	0.95	0.29
6	Butane	106-97-8	1.75	0.57
7	2-Methyl-1-Propene	115-11-7	0.26	0.08
8	Ethanol	64-17-5	0.19	0.06
9	2-Methyl-1-Butene	563-46-2	0.11	0.05
10	Isopropyl Alcohol ³	67-63-0	0.17	--
11	1-Pentene	109-67-1	0.59	0.33
12	Pentane	109-66-0	1.57	0.66
13	2-methyl-2-Propanol	75-65-0	0.10	0.03
14	4-Methyl-1-Pentene	691-37-2	0.16	0.04
15	2-Methylpentane	107-83-5	1.19	0.30
16	Butanal	123-72-8	0.13	0.04
17	3-Methylpentane	96-14-0	0.24	0.06
18	1-Hexene	592-41-6	0.20	0.05
19	Methylcyclopentane	96-37-7	0.15	0.04
20	Unknown Ketone		0.14	0.01
21	1-Butanol	71-36-3	0.59	0.04
22	2-Pentanone	107-87-9	0.81	0.06
23	Unknown C7 Alkane		0.48	0.01
24	1-Heptene	592-76-7	0.13	0.00
25	Unknown Alcohol ²		0.08	--
26	Unknown		0.07	0.00
27	Unknown C8 Alkane		0.29	0.00

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
28	2-Hexanone	591-78-6	0.29	0.01
29	Octane	111-65-9	0.27	0.00
30	Unknown C9 Alkane		0.10	0.00
31	Unknown C9 Alkene/Cycloalkane		0.06	0.00
32	3-Heptanone	106-35-4	0.42	0.01
33	2-Heptanone	110-43-0	0.23	0.00
34	Nonane	111-84-2	0.20	0.00
35	Unknown Ketone		0.24	0.01
36	2-Octanone	111-13-7	0.07	0.01
37	Unknown C11 Alkane		0.13	0.01
38	Unknown C10 Alkene/Cycloalkane		0.09	0.02
39	Undecane	1120-21-4	0.37	0.03
40	Unknown C11 Alkene/Cycloalkane ³		0.07	--
41	Unknown C12 Alkane ³		0.07	--
42	Dodecane	112-40-3	0.54	0.04
43	Undecane, 2,6-dimethyl-	17301-23-4	0.27	0.02
44	Unknown C13 Alkene/Cycloalkane		0.15	0.02
45	Unknown C14 Alkane		0.30	0.02
46	Tridecane	629-50-5	0.48	0.04
47	Unknown C14 Alkane		0.07	0.00
48	Unknown C13 Alkene/Cycloalkane		0.07	0.00
49	Unknown C15 Alkane		0.21	0.02
50	Tetradecane	629-59-4	0.25	0.02
Sum of tentatively identified compounds:			18.92	

1 CAS = Chemical Abstract Service.

2 Average of three samples, values listed are estimates.

3 Detected in only 1 sample.

Table 4-7
 Tank BY-110 Tentatively Identified Organic Compounds in TST Samples
 in the Order of Chromatographic Elution --
 Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Isobutane	75-28-5	0.24	0.09
2	1-Propene, 2-methyl-	115-11-7	0.44	0.05
3	Butane	106-97-8	1.4	0.4
4	1-Propene, 2-methyl-	115-11-7	0.11	0.03
5	1-Butene	106-98-9	0.053	0.054
6	2-Butene	107-01-7	0.042	0.072
7	1-Butene	106-98-9	0.015	0.026
8	Cyclopropane, 1,2-dimethyl-, trans-	2402-06-4	0.032	0.028
9	1-Butene, 2-methyl-	563-46-2	0.020	0.034
10	Butane, 2-methyl-	78-78-4	0.61	0.003
11	Trichloromonofluoromethane	75-69-4	0.13	0.006
12	1-Pentene	109-67-1	0.22	0.009
13	1,3-Pentadiene, (Z)	1574-41-0	0.084	0.015
14	Isopropyl Alcohol	67-63-0	0.17	0.09
15	1-Pentene	109-67-1	0.042	0.008
16	1-Hexene	592-41-6	0.070	0.012
17	Pentane, 2-methyl-	107-83-5	0.53	0.05
18	1-Propanol	71-23-8	0.18	0.04
19	Pentane, 3-methyl-	96-14-0	0.095	0.009
20	1-Hexene	592-41-6	0.10	0.002
21	2-Butanone	78-93-3	0.22	0.10
22	1-Hexanol	111-27-3	0.029	0.050
23	Cyclohexane	110-82-7	0.019	0.033
24	Furan, tetrahydro-	109-99-9	0.19	0.13
25	Hexane, 2-methyl-	591-76-4	0.10	0.01
26	Hexane, 3-methyl-	589-34-4	0.31	0.03
27	1-Heptene	592-76-7	0.030	0.026

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
28	3-Pentanone	96-22-0	0.042	0.003
29	2-Butanone, 3,3-dimethyl-	75-97-8	0.051	0.004
30	Cyclohexane, methyl-	108-87-2	0.079	0.006
31	Methyl Isobutyl Ketone	108-10-1	0.074	0.003
32	Pentane, 2-cyclopropyl-	5458-16-2	0.010	0.017
33	Heptane, 3-methyl-	589-81-1	0.055	0.048
34	Cyclohexane, 1,3-dimethyl-, cis-	638-04-0	0.022	0.038
35	1-Pentanol	71-41-0	0.033	0.057
36	3-Hexanone	589-38-8	0.037	0.004
37	Methanamine, N-(1-methylbutylidene)-	22431-09-0	0.015	0.026
38	Heptane, 2,6-dimethyl-	1072-05-5	0.040	0.005
39	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.041	0.004
40	2-Hexanone, 4-methyl-	105-42-0	0.027	0.024
41	1-Hexanol	111-27-3	0.088	0.004
42	4-Heptanone & C2 Benzene		0.085	0.005
43	3-Heptanone	106-35-4	0.41	0.02
44	2-Heptanone, 6-methyl-	928-68-7	0.036	0.002
45	1H-Indene, octahydro-, cis-	4551-51-3	0.037	0.010
46	Octane, 2,6-dimethyl-	2051-30-1	0.029	0.025
47	Cyclohexane, propyl-	1678-92-8	0.045	0.002
48	1,4-Pentadien-3-ol	922-65-6	0.009	0.016
49	2-Heptanone, 6-methyl-	928-68-7	0.18	0.01
50	Nonane, 4-methyl-	17301-94-9	0.038	0.002
51	Cyclohexane, 1,1,2,3-tetramethyl-	6783-92-2	0.10	0.01
52	1-Heptanol	111-70-6	0.048	0.006
53	Cyclotetrasiloxane, octamethyl-	556-67-2	0.011	0.019
54	Cyclohexane, 1-methyl-2-propyl-	4291-79-6	0.042	0.009
55	Cyclohexane, 1-methyl-2-propyl-	4291-79-6	0.017	0.016
56	2-Nonenal, (E)-	18829-56-6	0.006	0.011

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
57	Nonane, 2,6-dimethyl-	17302-28-2	0.083	0.004
58	Limonene	138-86-3	0.006	0.011
59	Cyclohexane, butyl-	1678-93-9	0.027	0.001
60	Cyclopropane, 1,2-dibutyl-	41977-32-6	0.042	0.001
61	Heptane, 2,6-dimethyl-	1072-05-5	0.026	0.001
62	2-Heptanone, 6-methyl-	928-68-7	0.013	0.012
63	Undecane, 3,4-dimethyl-	17312-78-6	0.020	0.001
64	Naphthalene, decahydro-, trans-	493-02-7	0.027	0.0003
65	Cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.077	0.003
66	C5-cyclohexane		0.058	0.003
67	Undecane, 3,7-dimethyl-	17301-29-0	0.042	0.002
68	methyl-decahydronaphthalene		0.016	0.028
69	Undecane, 4,8-dimethyl-	17301-33-6	0.016	0.028
70	Undecane, 4,7-dimethyl-	17301-32-5	0.015	0.026
71	Decane, 2,3,8-trimethyl-	62238-14-6	0.017	0.029
72	Naphthalene, decahydro-2-methyl-	2958-76-1	0.035	0.031
73	Cyclohexane, pentyl-	4292-92-6	0.072	0.003
74	Naphthalene, decahydro-2-methyl-	2958-76-1	0.059	0.002
75	Decane, 2,5-dimethyl-	17312-50-4	0.051	0.003
76	Decane, 3-methyl-	13151-34-3	0.032	0.003
77	Nonane, 5-(2-methylpropyl)-	62185-53-9	0.057	0.002
78	Decane, 3,8-dimethyl-	17312-55-9	0.042	0.0004
79	Naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.028	0.004
80	3-Dodecene, (E)-	7206-14-6	0.015	0.013
81	Naphthalene, decahydro-2,6-dimethyl	1618-22-0	0.031	0.010
82	Naphthalene, decahydro-1,5-dimethyl	66552-62-3	0.029	0.003
83	C6-cyclohexane		0.029	0.004
84	Undecane, 2,6-dimethyl-	17301-23-4	0.25	0.01
85	Dodecane, 5-methyl- & others		0.036	0.004

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
86	Naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.042	0.004
87	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.075	0.002
88	Cyclohexane, hexyl-	4292-75-5	0.18	0.01
89	Dodecane, 4-methyl-	6117-97-1	0.042	0.004
90	Decane, 2,3,7-trimethyl-	62238-13-5	0.057	0.004
91	Cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.029	0.002
92	Tridecane, 7-methyl-	26730-14-3	0.30	0.02
93	Cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.028	0.003
94	Cyclopentene, 5-hexyl-3,3-dimethyl-	61142-66-3	0.027	0.001
95	Undecane, 3,9-dimethyl-	17301-31-4	0.088	0.001
96	Tridecane, 6-methyl-	13287-21-3	0.007	0.012
97	Cyclohexane, octyl-	1795-15-9	0.081	0.003
98	Tridecane, 2-methyl-	1560-96-9	0.047	0.002
99	Decane, 3,8-dimethyl-	17312-55-9	0.037	0.003
100	Dodecane, 2,6,11-trimethyl-	31295-56-4	0.33	0.02
101	Tetradecane	629-59-4	0.40	0.02
102	Tridecane, 4,8-dimethyl-	55030-62-1	0.047	0.004
103	C9-cyclohexane		0.043	0.002
104	Hexadecane	544-76-3	0.20	0.01
105	Pentadecane	629-62-9	0.16	0.01
106	Pentadecane, 2-methyl-	1560-93-6	0.006	0.011
107	Hexadecane	544-76-3	0.016	0.014
108	Tetradecanoic acid	544-63-8	0.043	0.022
109	Benzenesulfonamide, N-butyl-	3622-84-2	0.17	0.02
110	1-Heptadecanol	1454-85-9	0.008	0.014
111	Hexadecanoic acid	57-10-3	0.043	0.046
Sum of tentatively identified compounds:			10.91	

1 CAS = Chemical Abstract Service

2 Average of 4 TST samples by ORNL: 3 were 250 ml and 1 was 50 ml, values listed are estimates.

Table 4-8
 Tank BY-110 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)
22	1-Hexanol	111-27-3	0.029	0.050
2	1-Propene, 2-methyl-	115-11-7	0.44	0.05
52	1-Heptanol	111-70-6	0.048	0.006
4	1-Propene, 2-methyl-	115-11-7	0.11	0.03
5	1-Butene	106-98-9	0.053	0.054
20	1-Hexene	592-41-6	0.10	0.002
7	1-Butene	106-98-9	0.015	0.026
18	1-Propanol	71-23-8	0.18	0.04
9	1-Butene, 2-methyl	563-46-2	0.020	0.034
27	1-Heptene	592-76-7	0.030	0.026
41	1-Hexanol	111-27-3	0.088	0.004
12	1-Pentene	109-67-1	0.22	0.009
35	1-Pentanol	71-41-0	0.033	0.057
110	1-Heptadecanol	1454-85-9	0.008	0.014
15	1-Pentene	109-67-1	0.042	0.008
16	1-Hexene	592-41-6	0.070	0.012
13	1,3-Pentadiene, (Z)	1574-41-0	0.084	0.015
48	1,4-Pentadien-3-ol	922-65-6	0.009	0.016
45	1H-Indene, octahydro-, cis-	4551-51-3	0.037	0.010
6	2-Butene	107-01-7	0.042	0.072
21	2-Butanone	78-93-3	0.22	0.10
62	2-Heptanone, 6-methyl-	928-68-7	0.013	0.012
40	2-Hexanone, 4-methyl-	105-42-0	0.027	0.024
29	2-Butanone, 3,3-dimethyl-	75-97-8	0.051	0.004
56	2-Nonenal, (E)-	18829-56-6	0.006	0.011
44	2-Heptanone, 6-methyl-	928-68-7	0.036	0.002
49	2-Heptanone, 6-methyl-	928-68-7	0.18	0.01

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
28	3-Pentanone	96-22-0	0.042	0.003
80	3-Dodecene, (E)-	7206-14-6	0.015	0.013
43	3-Heptanone	106-35-4	0.41	0.02
36	3-Hexanone	589-38-8	0.037	0.004
42	4-Heptanone & C2 Benzene		0.085	0.005
109	Benzenesulfonamide, N-butyl-	3622-84-2	0.17	0.02
3	Butane	106-97-8	1.4	0.4
10	Butane, 2-methyl-	78-78-4	0.61	0.003
66	C5-cyclohexane		0.058	0.003
83	C6-cyclohexane		0.029	0.004
103	C9-cyclohexane		0.043	0.002
23	Cyclohexane	110-82-7	0.019	0.033
30	Cyclohexane, methyl-	108-87-2	0.079	0.006
34	Cyclohexane, 1,3-dimethyl-, cis-	638-04-0	0.022	0.038
39	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.041	0.004
47	Cyclohexane, propyl-	1678-92-8	0.045	0.002
51	Cyclohexane, 1,1,2,3-tetramethyl-	6783-92-2	0.10	0.01
54	Cyclohexane, 1-methyl-2-propyl-	4291-79-6	0.042	0.009
55	Cyclohexane, 1-methyl-2-propyl-	4291-79-6	0.017	0.016
59	Cyclohexane, butyl-	1678-93-9	0.027	0.001
65	Cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.077	0.003
73	Cyclohexane, pentyl-	4292-92-6	0.072	0.003
87	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.075	0.002
88	Cyclohexane, hexyl-	4292-75-5	0.18	0.01
91	Cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.029	0.002
93	Cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.028	0.003
97	Cyclohexane, octyl-	1795-15-9	0.081	0.003
94	Cyclopentene, 5-hexyl-3,3-dimethyl-	61142-66-3	0.027	0.001
8	Cyclopropane, 1,2-dimethyl-, trans-	2402-06-4	0.032	0.028

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
60	Cyclopropane, 1,2-dibutyl-	41977-32-6	0.042	0.001
53	Cyclotetrasiloxane, octamethyl-	556-67-2	0.011	0.019
71	Decane, 2,3,8-trimethyl-	62238-14-6	0.017	0.029
75	Decane, 2,5-dimethyl-	17312-50-4	0.051	0.003
76	Decane, 3-methyl-	13151-34-3	0.032	0.003
78	Decane, 3,8-dimethyl-	17312-55-9	0.042	0.0004
90	Decane, 2,3,7-trimethyl-	62238-13-5	0.057	0.004
99	Decane, 3,8-dimethyl-	17312-55-9	0.037	0.003
85	Dodecane, 5-methyl- & others		0.036	0.004
89	Dodecane, 4-methyl-	6117-97-1	0.042	0.004
100	Dodecane, 2,6,11-trimethyl-	31295-56-4	0.33	0.02
24	Furan, tetrahydro-	109-99-9	0.19	0.13
33	Heptane, 3-methyl-	589-81-1	0.055	0.048
38	Heptane, 2,6-dimethyl-	1072-05-5	0.040	0.005
61	Heptane, 2,6-dimethyl-	1072-05-5	0.026	0.001
104	Hexadecane	544-76-3	0.20	0.01
107	Hexadecane	544-76-3	0.016	0.014
111	Hexadecanoic acid	57-10-3	0.043	0.046
25	Hexane, 2-methyl-	591-76-4	0.10	0.01
26	Hexane, 3-methyl-	589-34-4	0.31	0.03
1	Isobutane	75-28-5	0.24	0.09
14	Isopropyl Alcohol	67-63-0	0.17	0.09
58	Limonene	138-86-3	0.006	0.011
37	Methanamine, N-(1-methylbutylidene)-	22431-09-0	0.015	0.026
68	methyl-decahydronaphthalene		0.016	0.028
31	Methyl Isobutyl Ketone	108-10-1	0.074	0.003
64	Naphthalene, decahydro-, trans-	493-02-7	0.027	0.0003
72	Naphthalene, decahydro-2-methyl-	2958-76-1	0.035	0.031
74	Naphthalene, decahydro-2-methyl-	2958-76-1	0.059	0.002

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
79	Naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.028	0.004
81	Naphthalene, decahydro-2,6-dimethyl-	1618-22-0	0.031	0.010
82	Naphthalene, decahydro-1,5-dimethyl-	66552-62-3	0.029	0.003
86	Naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.042	0.004
50	Nonane, 4-methyl-	17301-94-9	0.038	0.002
57	Nonane, 2,6-dimethyl-	17302-28-2	0.083	0.004
77	Nonane, 5-(2-methylpropyl)-	62185-53-9	0.057	0.002
46	Octane, 2,6-dimethyl-	2051-30-1	0.029	0.025
105	Pentadecane	629-62-9	0.16	0.01
106	Pentadecane, 2-methyl	1560-93-6	0.006	0.011
17	Pentane, 2-methyl-	107-83-5	0.53	0.05
19	Pentane, 3-methyl-	96-14-0	0.095	0.009
32	Pentane, 2-cyclopropyl-	5458-16-2	0.010	0.017
101	Tetradecane	629-59-4	0.40	0.02
108	Tetradecanoic acid	544-63-8	0.043	0.022
11	Trichloromonofluoromethane	75-69-4	0.13	0.006
92	Tridecane, 7-methyl-	26730-14-3	0.30	0.02
96	Tridecane, 6-methyl-	13287-21-3	0.007	0.012
98	Tridecane, 2-methyl-	1560-96-9	0.047	0.002
102	Tridecane, 4,8-dimethyl-	55030-62-1	0.047	0.004
63	Undecane, 3,4-dimethyl-	17312-78-6	0.020	0.001
67	Undecane, 3,7-dimethyl-	17301-29-0	0.042	0.002
69	Undecane, 4,8-dimethyl-	17301-33-6	0.016	0.028
70	Undecane, 4,7-dimethyl-	17301-32-5	0.015	0.026
84	Undecane, 2,6-dimethyl-	17301-23-4	0.25	0.01
95	Undecane, 3,9-dimethyl-	17301-31-4	0.088	0.001
Sum of tentatively identified compounds:			10.91	

1 CAS = Chemical Abstract Service

2 Average of 4 TST samples by ORNL: 3 were 250 ml and 1 was 50 ml, values listed are estimates.

Table 4-9
 Tank BY-110 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)
3	Butane	106-97-8	1.4	0.4
10	Butane, 2-methyl-	78-78-4	0.61	0.003
17	Pentane, 2-methyl-	107-83-5	0.53	0.05
2	1-Propene, 2-methyl-	115-11-7	0.44	0.05
43	3-Heptanone	106-35-4	0.41	0.02
101	Tetradecane	629-59-4	0.40	0.02
100	Dodecane, 2,6,11-trimethyl-	31295-56-4	0.33	0.02
26	Hexane, 3-methyl-	589-34-4	0.31	0.03
92	Tridecane, 7-methyl-	26730-14-3	0.30	0.02
84	Undecane, 2,6-dimethyl-	17301-23-4	0.25	0.01
1	Isobutane	75-28-5	0.24	0.09
12	1-Pentene	109-67-1	0.22	0.009
21	2-Butanone	78-93-3	0.22	0.10
104	Hexadecane	544-76-3	0.20	0.01
24	Furan, tetrahydro-	109-99-9	0.19	0.13
49	2-Heptanone, 6-methyl-	928-68-7	0.18	0.01
88	Cyclohexane, hexyl-	4292-75-5	0.18	0.01
18	1-Propanol	71-23-8	0.18	0.04
109	Benzenesulfonamide, N-butyl-	3622-84-2	0.17	0.02
14	Isopropyl Alcohol	67-63-0	0.17	0.09
105	Pentadecane	629-62-9	0.16	0.01
11	Trichloromonofluoromethane	75-69-4	0.13	0.006
4	1-Propene, 2-methyl-	115-11-7	0.11	0.03
20	1-Hexene	592-41-6	0.10	0.002
25	Hexane, 2-methyl-	591-76-4	0.10	0.01
51	Cyclohexane, 1,1,2,3-tetramethyl-	6783-92-2	0.10	0.01
19	Pentane, 3-methyl-	96-14-0	0.095	0.009

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
95	Undecane, 3,9-dimethyl-	17301-31-4	0.088	0.001
41	1-Hexanol	111-27-3	0.088	0.004
42	4-Heptanone & C2 Benzene		0.085	0.005
13	1,3-Pentadiene, (Z)	1574-41-0	0.084	0.015
57	Nonane, 2,6-dimethyl-	17302-28-2	0.083	0.004
97	Cyclohexane, octyl-	1795-15-9	0.081	0.003
30	Cyclohexane, methyl-	108-87-2	0.079	0.006
65	Cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.077	0.003
87	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.075	0.002
31	Methyl Isobutyl Ketone	108-10-1	0.074	0.003
73	Cyclohexane, pentyl-	4292-92-6	0.072	0.003
16	1-Hexene	592-41-6	0.070	0.012
74	Naphthalene, decahydro-2-methyl-	2958-76-1	0.059	0.002
66	C5-cyclohexane		0.058	0.003
77	Nonane, 5-(2-methylpropyl)-	62185-53-9	0.057	0.002
90	Decane, 2,3,7-trimethyl-	62238-13-5	0.057	0.004
33	Heptane, 3-methyl-	589-81-1	0.055	0.048
5	1-Bufene	106-98-9	0.053	0.054
75	Decane, 2,5-dimethyl-	17312-50-4	0.051	0.003
29	2-Butanone, 3,3-dimethyl-	75-97-8	0.051	0.004
52	1-Heptanol	111-70-6	0.048	0.006
98	Tridecane, 2-methyl-	1560-96-9	0.047	0.002
102	Tridecane, 4,8-dimethyl-	55030-62-1	0.047	0.004
47	Cyclohexane, propyl-	1678-92-8	0.045	0.002
111	Hexadecanoic acid	57-10-3	0.043	0.046
108	Tetradecanoic acid	544-63-8	0.043	0.022
103	C9-cyclohexane		0.043	0.002
54	Cyclohexane, 1-methyl-2-propyl-	4291-79-6	0.042	0.009
15	1-Pentene	109-67-1	0.042	0.008

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
86	Naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.042	0.004
6	2-Butene	107-01-7	0.042	0.072
89	Dodecane, 4-methyl-	6117-97-1	0.042	0.004
60	Cyclopropane, 1,2-dibutyl-	41977-32-6	0.042	0.001
78	Decane, 3,8-dimethyl-	17312-55-9	0.042	0.0004
67	Undecane, 3,7-dimethyl-	17301-29-0	0.042	0.002
28	3-Pentanone	96-22-0	0.042	0.003
39	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.041	0.004
38	Heptane, 2,6-dimethyl-	1072-05-5	0.040	0.005
50	Nonane, 4-methyl-	17301-94-9	0.038	0.002
99	Decane, 3,8-dimethyl-	17312-55-9	0.037	0.003
36	3-Hexanone	589-38-8	0.037	0.004
45	1H-Indene, octahydro-, cis-	4551-51-3	0.037	0.010
85	Dodecane, 5-methyl- & others		0.036	0.004
44	2-Heptanone, 6-methyl-	928-68-7	0.036	0.002
72	Naphthalene, decahydro-2-methyl-	2958-76-1	0.035	0.031
35	1-Pentanol	71-41-0	0.033	0.057
8	Cyclopropane, 1,2-dimethyl-, trans-	2402-06-4	0.032	0.028
76	Decane, 3-methyl-	13151-34-3	0.032	0.003
81	Naphthalene, decahydro-2,6-dimethyl-	1618-22-0	0.031	0.010
27	1-Heptene	592-76-7	0.030	0.026
91	Cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.029	0.002
22	1-Hexanol	111-27-3	0.029	0.050
83	C6-cyclohexane		0.029	0.004
46	Octane, 2,6-dimethyl-	2051-30-1	0.029	0.025
82	Naphthalene, decahydro-1,5-dimethyl-	66552-62-3	0.029	0.003
93	Cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.028	0.003
79	Naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.028	0.004
59	Cyclohexane, butyl-	1678-93-9	0.027	0.001

WHC-SD-WM-ER-429 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
64	Naphthalene, decahydro-, trans-	493-02-7	0.027	0.0003
40	2-Hexanone, 4-methyl-	105-42-0	0.027	0.024
94	Cyclopentene, 5-hexyl-3,3-dimethyl-	61142-66-3	0.027	0.001
61	Heptane, 2,6-dimethyl-	1072-05-5	0.026	0.001
34	Cyclohexane, 1,3-dimethyl-, cis-	638-04-0	0.022	0.038
9	1-Butene, 2-methyl-	563-46-2	0.020	0.034
63	Undecane, 3,4-dimethyl-	17312-78-6	0.020	0.001
23	Cyclohexane	110-82-7	0.019	0.033
71	Decane, 2,3,8-trimethyl-	62238-14-6	0.017	0.029
55	Cyclohexane, 1-methyl-2-propyl-	4291-79-6	0.017	0.016
107	Hexadecane	544-76-3	0.016	0.014
68	methyl-decahydronaphthalene		0.016	0.028
69	Undecane, 4,8-dimethyl-	17301-33-6	0.016	0.028
80	3-Dodecene, (E)-	7206-14-6	0.015	0.013
7	1-Butene	106-98-9	0.015	0.026
70	Undecane, 4,7-dimethyl-	17301-32-5	0.015	0.026
37	Methanamine, N-(1-methylbutylidene)-	22431-09-0	0.015	0.026
62	2-Heptanone, 6-methyl-	928-68-7	0.013	0.012
53	Cyclotetrasiloxane, octamethyl-	556-67-2	0.011	0.019
32	Pentane, 2-cyclopropyl-	5458-16-2	0.010	0.017
48	1,4-Pentadien-3-ol	922-65-6	0.009	0.016
110	1-Heptadecanol	1454-85-9	0.008	0.014
96	Tridecane, 6-methyl-	13287-21-3	0.007	0.012
56	2-Nonenal, (E)-	18829-56-6	0.006	0.011
58	Limonene	138-86-3	0.006	0.011
106	Pentadecane, 2-methyl-	1560-93-6	0.006	0.011
Sum of tentatively identified compounds:			10.91	

¹ CAS = Chemical Abstract Service

² Average of 4 TST samples by ORNL: 3 were 250 ml and 1 was 50 ml, values listed are estimates.